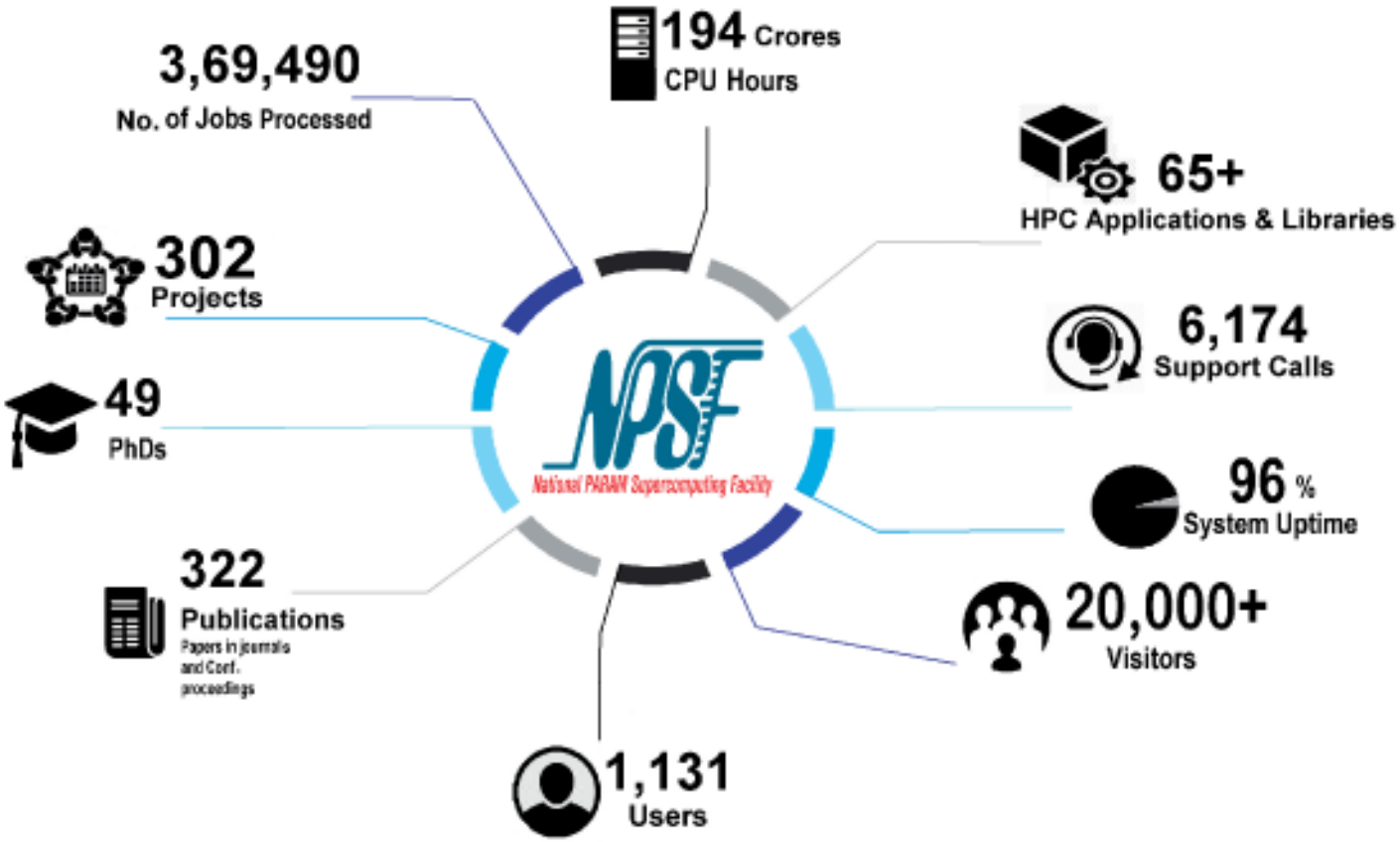
National PARAM Supercomputing Facility

ANNUAL REPORT
2018



Version 2.0

सी-डैक
CDAC
CENTRE FOR DEVELOPMENT OF ADVANCED COMPUTING
www.cdac.in

Cover Note

Dear Reader,

Taking forward tradition, NPSF is proud to presents Annual Report for the year 2018. The report put forth information so as to provide you with both qualitative and quantitative indices of work carried out using NPSF's HPC-As-A-Services, with an intention to perceive and analyze, both our performance, and in general HPC percolation in INDIA. For the quantitative part, system utilization metrics recorded over the year are incorporated, presenting assorted views of varying utilization aspects. For qualitative part, more specifically the scientific outcome of utilization, we have participation from NPSF's user community wherein information regarding PhDs, Publications, Work Reports are included verbatim. For reason that from this year onward, report period has been adjusted to Jan-Dec cycle instead of Feb-Mar earlier, there is an overlap of three months between previous and current report.

We would highly appreciate your say on report attached and NPSF in toto, for which you may write to `npsfhelp@cdac.in` email address.

Regards
NPSF

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आवरण पत्र

प्रिय पाठक गण,

अपनी परंपरा को आगे बढ़ाते हुए, आपके अनुशीलन के लिए एनपीएसएफ अपनी वार्षिक रिपोर्ट प्रस्तुत करते हुए गौरवान्वित है। आप हमारे प्रदर्शन के साथ ही भारत में आम रूप से एचपीसी गतिविधियों को समझें और विश्लेषण करें, इसी अभिप्राय के साथ इस रिपोर्ट के माध्यम से एनपीएसएफ के एचपीसी को सेवाओं के रूप में उपयोग करते हुए संपादित कार्यों की गुणात्मक और परिमाणात्मक दोनों पहलुओं को प्रस्तुत किया जा रहा है। परिणात्मक भाग के रूप में, वर्ष के दौरान रिकॉर्ड किए गए प्रणाली उपयोगिता कार्यों को शामिल किया गया है, जिसमें विभिन्न उपयोगिता पहलुओं के समावेशी विचार हैं। गुणात्मक भाग के रूप में, विशेष रूप से उपयोगिता के वे वैज्ञानिक परिणाम शामिल हैं, जो हमारे द्वारा एनपीएसएफ उपयोगकर्ता समुदाय से प्रतिभागिता के रूप में हुए हैं। इसमें शब्दशः पीएचडी, प्रकाशन कार्य, कार्य रिपोर्ट के बारे में जानकारी शामिल है। इस वर्ष से रिपोर्ट की अवधि जनवरी-दिसंबर चक्र के रूप में समायोजित की गई है, जो पहले फरवरी-मार्च के रूप में समायोजित होती थी और इस कारण से पूर्व के और वर्तमान रिपोर्ट में तीन महीने का ओवरलैप है।

हमें अति प्रसन्नता होगी, यदि आप संलग्न रिपोर्ट और एनपीएसएफ पर अपने अमूल्य विचार/ प्रतिक्रिया से हमें अवगत कराते हैं, इसके लिए आप हमें **npsfhelp@cdac.in** पर ईमेल कर सकते हैं।

भवदीय

एनपीएसएफ

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Dr. Hemant Darbari
Director General, C-DAC

Message from Director General

My memories go way back to the Year 2013, a major mile stone in the history of NPSF. The launch of PARAM Yuva II, a paradigm shift towards 1^st hybrid and by far most power efficient HPC system in the country, ranked in both Top 500 and Green 500 list of supercomputers of the world. Since then, NPSF has been the trend setter in INDIA with leading HPC resource utilization and for that matter uptime of the HPC services to the tune of 96%.

For all the successive years 2013 onwards, each year NPSF saw the ever increasing demand for the HPC resources with a record execution of >350 thousand HPC jobs under 200 Projects submitted by 1000+ users from across 100+ academic and research institutions.

These encouraging figures over the years helped in culminating the idea of having multiple and many fold HPC facilities in the country through National Super Computing Mission (NSM). Recent launch of PARAM Shivay, 833 TeraFlop HPC system by Honorable Prime Minister Shri. Narendra Modi speaks out the importance of this Mission and the commitment of C-DAC towards Research initiatives in the country and also asserts C-DAC's competence in leader's position in INDIA for all the verticals of HPC.

Education and Research are the backbone of the country. NPSF is unique in India offering High Performance Computing right from student to the researcher. It is evident that application of HPC has encompassed multitude of scientific & research domains as is not confined to Weather Research & Forecasting (WRF), provenance of HPC in INDIA. Lately demands of new application areas like AI using ML/DL approach coupled with mainstream field of big data analytics.

At last, I would like to congratulate NPSF team of C-DAC, Pune for their achievements and relentless efforts in running the facility and their contributions to the mission and that insightful reports like this continue for years to come.

Dr. Hemant Darbari
Director General, C-DAC

Col. A. K. Nath (Retd.)
Executive Director, C-DAC, Pune

Message from Executive Director

Computational tools offer society a new problem solving paradigm. They have the potential to provide accurate predictions of complex phenomena for realistic conditions. These tools offer the potential to rapidly produce optimized designs for systems, explore the limits of those designs, accelerate scientific discoveries, predict the behaviour of natural systems like the weather, analyse and plan complex operations involving thousands to millions of individual entities, and analyse & organize enormous amounts of data.

This year PARAM Yuva-II completed 6 years of serving the supercomputing community of the nation. Since its commissioning, the National PARAM Supercomputing Facility (NPSF) has catered to more than 1131 users from around 114 scientific institutions.

I thank all users of NPSF for their incessant support and their excellent contribution towards the Academic and Scientific community. The enriching experience earned throughout the journey has equipped C-DAC facing various computational challenges. C-DAC, Pune is happy to share a new feather in its cap, 'PARAM Shivay' under C-DAC's flagship project, National Supercomputing Mission (NSM) which was inaugurated by Honourable Prime Minister, Shri. Narendra Modi on February 19, 2019 at IIT (BHU), Varanasi.

Collaboration with premier Scientific & engineering organisations will certainly help HPC team @ C-DAC in overcoming the challenges related to development of next generation exascale systems development.

I wish you all the success for your future endeavours!

Col. A. K. Nath (Retd.)
Executive Director
C-DAC, Pune

;

Vinodh Kumar M.
Senior Director & HoD,
HPC-I&E Group, C-DAC, Pune

Message from Head of Department

NPSF has entered its twenty-first year of operations with its seven-year-old PARAM Yuva-II; it is the longest running HPC system in the PARAM series of supercomputers. NPSF has continuously increased system performance metrics - in a multitude of characteristics of assessment - both quantitatively and qualitatively, as reported annually in these reports. Governmental bodies, funding agencies, and policy makers are able to carry out a comprehensive assessment of NPSF's performance while these reports also serve as a consistent source of structured information on HPC percolation in India.

For the latter, as a starter, a visible geographic distribution of usage, users and institutes together with scientific outcome (PhDs and publications) has been presented on the India map, giving the reader a graphical view of the pervasiveness of HPC across the country.

Scientific work conceived and incepted using NPSF's HPC services in 2018 has seen a substantial increase. There has also been an increase in publications being reported during the same time.

With a 99.95% availability during year 2018, NPSF has re-emphasized it's resolve to serve the nation to its fullest capability. However, this has not been an easy task for our team, the seven-year-old PARAM Yuva-II ecosystem is now extremely prone to hardware and other failures as it is nearing its end-of-life.

NPSF has also started generation of CPU utilization reports to sensitize the user community on the value and cost of the services and facilities used by them. This is to underline the reality that it is tremendously expensive to keep any HPC facility operational, and also that such services cannot be taken for granted, or to be available for free for much too long.

Vinodh Kumar M.
Senior Director & HoD,
HPC-I&E Group, C-DAC, Pune

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INDIAN INSTITUTE OF SCIENCE EDUCATION AND RESEARCH PUNE
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जयंत बी. उदगांवकर *प्राध्यापक एवं निदेशक*
Jayant B. Udgaonkar *Professor and Director*

March 30, 2019

To whomsoever concerned

IISER-Pune would like to acknowledge the National PARAM Supercomputing Facility (NPSF) at CDAC Pune, and would also like to express our special gratitude to the NPSF-team, who have been maintaining such an excellent national facility. Researchers at IISER-Pune including the PhD students and postdocs are relentlessly using the facility for their research in various cutting-edge topics such as heterogeneous catalysis, thermoelectrics, nuclear quantum effects, photocatalytic water splitting, two-dimensional and quantum materials etc. During the last one year, our researchers have published as many as 11 papers, and 3 of our PhD students have submitted their thesis based on work using the NPSF facility, which would not have been possible without it. In every form of scientific dissemination, we acknowledge the generous support that CDAC is extending to us over many years. We sincerely hope that our successful collaboration with CDAC will be sustained in future.

(Prof. Jayant B. Udgaonkar)
Director

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नैनो विज्ञान एवं प्रौद्योगिकी संस्थान

(विज्ञान एवं प्रौद्योगिकी विभाग, भारत सरकार का एक स्वायत्त संस्थान)

Institute of Nano Science and Technology

(An Autonomous Institute of Department of Science & Technology, Govt. of India)

प्रो. हीरेन्द्र नाथ घोष
निदेशक (कार्यवाहक)
Prof. Hirendra Nath Ghosh FASc FNASc FNA
Director (offg)

F.No. 31(1)/2019-INST

Dated 1st April, 2019

To

Shri Rishi Pathak
Principal Technical Officer
National PARAM Supercomputing Facility **(NPSF)**
Centre for Development of Advanced Computing **(C-DAC)**
Ganeshkhind Road, Pune University Campus, PUNE-Maharastra

Dear Sir,

Thank you for your kind email dated 22nd March, 2019

CDAC, Pune has been doing a wonderful job for many years in helping Computational Scientists across India in their active pursuit of research. The strong computational support provided by CDAC-Pune on PARAM Yuva II has helped our Computational Nano-scientists immensely in guiding their Ph.D. students and Postdocs on a wide range of research problems, and also in providing the experimentalists here with strong theoretical support. The helpdesk has responded with great promptitude in installing different programs & modules required by our Scientists from time to time. In short, helpdesk has been remarkably supportive. INST owes the deepest debt of gratitude to CDAC-Pune and the support team of PARAM Yuva II. PARAM Yuva II has brought to INST many Publications in prestigious journals.

Research on 2D materials conducted by Dr. Abir De Sarkar using the supercomputing resources on PARAM Yuva II has truly been recognized. CNR Rao Award for excellence in Nanoresearch for the year 2018 has been conferred upon him. His student, Ms Ashima Rawat, has been the recipient of the Best Poster Award at the ACS sponsored Conference on International Conference on Advances in Nanomaterials and Devices for Energy and Environment (ICAN-2019) held at IIITM, Gwalior in January, 2019.

We would like to appeal to the Govt. of India to allocate substantial funds to CDAC-Pune to support the latter in their future endeavors, which includes upgrading their HPC systems. Any HPC system gets outdated in five years. Moreover, the usage of Param Yuva II is extremely high. Param Yuva II caters to users from all over India. CDAC-Pune is in dire need of a strong funding support from the Govt. of India. Integration of the latest computational resources into the current HPC system is the crying need of the hour.

Wishing you continued success in your earnest endeavors.

Yours sincerely,

(Prof. H.N. Ghosh)

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Devang V. Khakhar, Director
देवांग वि. खक्खर, निदेशक

D.No.III/C-11/2019
April 04, 2019

Dear Shri Pathak,

Thank you for your email dated March 28, 2019, regarding the discernible impact of C-DAC's HPC-as-a-service facility made available to IIT Bombay. Firstly, greetings on the event of your Foundation Day.

Based on the feedback received from the user community, the following are the outcomes:

1. Number of Projects that used Param Yuva II: 9
2. Number of Publications in International Journals: 11
3. Number of students trained: 20

Comments on the usage by the faculty members is attached as an appendix.

With warm regards,

Yours sincerely,

[Devang Khakhar]

Shri Rishi Pathak,
Principal Technical Officer,
National Param Supercomputing Facility (NPSF)
Centre for Development of Advanced Computing (C-DAC)
Ganeshkhind Road, Pune University Campus
Pune – Maharashtra

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Office of the Director

IIT Bombay

Appendix

User Feedback

We have used it for doing MD simulations. It was extremely useful.
Kindly fix the number of cores per user because some users submit jobs using maximum number of cores and some has to wait for a long time.
We have used C-DAC cluster for abinit, paradis and LAMMPS calculations. Several theses have been based on the work done using this facility.
The Param Yuva facility was requested for a parallel computation project I was working on. The student who worked on it had many difficulties due to software compatibility issues and reported a very small actual time of use. The student later left before completing the work. I have not followed up further use of Param since over one year. I have informed by reply mail several times that I am not using Param Yuva anymore. My name may kindly be taken off the list of users. If I need the facility again in future and have a person who can make use of Param Yuva I shall request for an account again. Thank you for having offered the facility.
C-DAC uses CentOS 6.2 with GNU compilers version 4.4.2, which is old. At present, they provide higher versions of GNU compilers as a parallel install separately, which needs to be invoked each time you run the application requiring those higher versions of the compilers. It would be good if they could upgrade the OS and the compilers as a whole.
Have not used much in the past year.
My research has moved away from HPC. One MTech used Param Yuva for his project simulations.
Well-maintained useful resource. Please install emacs as an default editor besides vi.
If possible try to allocate fix number of cores to all users. Because some users are using a large number of cores while some has their jobs running on less number of cores and sometimes to wait for long.
Excellent facility...

भारतीय ताराभौतिकी संस्थान
INDIAN INSTITUTE OF ASTROPHYSICS

विज्ञान व प्रौद्योगिकी विभाग, भारत सरकार के अधीन स्वायत्त निकाय

(An Autonomous Body under Department of Science and Technology, Government of India)

II ब्लॉक Block, कोरमंगला Koramangala, बेंगलूरु Bengaluru - 560 034

आचार्य जयंत मूर्ति/**Prof. Jayant Murthy**
वरिष्ठ आचार्य & प्रभारी निदेशक / **Senior Professor & Director(A)**

फोन/Phone : 080 25530583
फैक्स/Fax : 080 25534019
ईमेल/Email : diriia@iiap.res.in

IIA.D.8825
April 15, 2019

To,
Mr. Rishi Pathak,
Principal Technical Officer,
National Param Supercomputing Facility
Centre for Development of Advanced Computing,
Ganeshkhind Road, Pune

Dear Mr. Rishi,

I am pleased to write this letter of acknowledgement. Since the beginning of 2016, two of our faculty members - Dr. Sharanya Sur and Dr. Piyali Chatterjee have been using CDAC's Param Yuva II supercomputer through the technical affiliation scheme (TAS). Their research project titled 'Hydromagnetic-Turbulence-PR' focusses on complex, numerical simulations of magnetohydrodynamic turbulence in the context of the Sun, galaxies and galaxy clusters and requires large scale high performance computing resources. The National Param Supercomputing Facility (NPSF) at CDAC was thus a natural choice as it offers academic members from different institutes to use supercomputing resources for their research through the TAS. With the help of computing time awarded at Param Yuva II over the last 3 years, I am happy to report that Dr. Sur and Dr. Chatterjee have explored a variety of research themes such as - the role of Fluctuation dynamos in young galaxies, decay of turbulence and magnetic fields in galaxy clusters, simulations of the solar atmosphere including the propagation of Alfven waves and coronal heating. Besides, significant time and effort has also been devoted for code development and testing. Their works have been published in peer-reviewed, high impact factor, international journals such as the 'Monthly Notices of the Royal Astronomical Society' and the 'Astrophysical Journal' and also reported in the annual work reports requested by CDAC. I am also aware that both Sharanya and Piyali have also presented these works in national and international conferences which concomitantly provides visibility to the supercomputing resources of CDAC.

We are grateful to CDAC's NPSF and in particular, the TAS which made it possible for our faculty members to utilise Param Yuva II for their research. While thanking the CDAC support staff for their service, we would like to suggest that support during critical technical issues related to supercomputing hardware be improved in a manner which does not affect the momentum and smooth work flow of the end user(s).

With best regards,

Sincerely,

Jayant Murthy

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SRI GURU GRANTH SAHIB WORLD UNIVERSITY
FATEHGARH SAHIB-140406 (PUNJAB), INDIA
ESTABLISHED BY PUNJAB STATE ACT 20/2008 & APPROVED UNDER SECTION 2(f) OF U.G.C. ACT, 1956

April 17, 2019

LETTER OF ACKNOWLEDGEMENT

Dr. Deepti Goyal and her research group members from Department of Chemistry, Sri Guru Granth Sahib World University (SGGSWU), Fatehgarh Sahib, Punjab, sincerely acknowledge National PARAM Supercomputing Facility (NPSF) for providing NPSF's HPC-As-A-Services. The computational facility is of great support for the Ph.D. as well as M.Sc. students to pursue their research projects and timely completion of the research work. The benefit of the NPSF is that the molecular dynamics simulations can be completed in short duration. The NPSF facility is easy to access and the staff at CDAC is very cooperative and quickly response to our queries. We thank the entire team of NPSF for their extended support and cooperation. The computational support provided by CDAC-Pune enables us to pursue good quality research and publish the work in peer-reviewed journals of international repute. The list of research papers published are as follows:

1. Impact of K16A and K28A mutation on the structure and dynamics of amyloid-β42 peptide in Alzheimer's disease: key insights from molecular dynamics simulations. S. Shuaib, R. K. Saini, D. Goyal, B. Goyal *J. Biomol. Struct. Dyn.* **2019**, doi.org/10.1080/07391102.2019.1586587.
2. Insights into the inhibitory mechanism of a resveratrol and clioquinol hybrid against $A\beta_{42}$ aggregation and protofibril destabilization: a molecular dynamics simulation study. R. K. Saini, S. Shuaib, D. Goyal, B. Goyal *J. Biomol. Struct. Dyn.* **2018**, doi. 10.1080/07391102.2018.
3. Molecular insights into the effect L17A/F19A double mutation on the structure and dynamics of Aβ40: a molecular dynamics simulation study. R. K. Saini, S. Shuaib, D. Goyal, B. Goyal *J. Cell. Biochem.* **2018**, 119, 8949.
4. Assessing the effect of D59P mutation in the DE loop region in amyloid aggregation propensity of β2-microglobulin: a molecular dynamics simulation study. S. S. Narang, S. Shuaib, D. Goyal, B. Goyal *J. Cell. Biochem.* **2018**, *119*, 782.

We thank CDAC-Pune for providing the computational support during last year in the project entitled "Inhibitors-Amyloid β-PR". We look forward to use the computational facility in near future for the benefit of students. On behalf of Department of Chemistry, SGGSWU, Fatehgarh Sahib, we sincerely appreciate the entire team of CDAC for providing the computational support and cooperation.

Signature of the PI
(Dr. Deepti Goyal)

17/4/19

Signature of Head of the Institute/Organisation
(Prof. Pritpal Singh)

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सरदार वल्लभभाई राष्ट्रीय प्रौद्योगिकी संस्थान, सूरत
SARDAR VALLABHBHAI NATIONAL INSTITUTE OF TECHNOLOGY, SURAT
સરદાર વલ્લભભાઈ રાષ્ટ્રીય પ્રૌદ્યોગિકી સંસ્થા, સુરત
SVNIT

To
Mr. Rishi Pathak
Principal Technical Officer
National PARAM Supercomputing Facility (NPSF)
Centre for Development of Advanced Computing (C-DAC)
PUNE

Date: April 18, 2019

Subject: Acknowledgement of the usage of National PARAM Supercomputing Facility (NPSF)

Dear Sir,

This is to acknowledge the usage of PARAM Yuva-II (HPC) of the National PARAM Supercomputing Facility (NPSF) of C-DAC, Pune by the following research groups in our Institute:

Project Name	CI Name
Potential-ClusterMotifs-PR	Dr. Debesh R. Roy, Applied Physics Dept
Novel-Perovskite-SolarCells-PR	Dr. Yogeshkumar Sonvane, Applied Physics Dept

The HPC facility is certainly benefiting the research activities of Dr. Roy and Dr. Sonvane in their area of Computational Materials Physics. The HPC support from the NPSF also helping the above research groups as well as our Institute, in terms publications of international repute.

We are sure that the support from C-DAC will be available in future as well.

I wish all the very best to the NPSF initiatives and their great success ahead.

Yours sincerely,

18/4/19

Prof. S. R. Gandhi
Director, SVNIT Surat

ICHCHHANATH, SURAT-395 007 (GUJARAT) INDIA
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Contents

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About NPSF

Clusters at NPSF

PARAM Yuva II: Operational from Year 2013, Peak Perf. 529.4 TFlop/s, Ranked 69^{th} in June 2013,Top500

PARAM Yuva: Operational Year 2008-2012, Peak Perf. 54 TFlop/s, Ranked 69^{th} in Nov. 2008,Top500

PARAM 10000: Operational Year 1998-2005,Peak Perf. 100 GFlop/s

1.1 Introduction

The National PARAM Supercomputing Facility (NPSF) is a result of more than two and half decade effort of Research and Development (R&D) in High Performance Computing (HPC) since C-DAC's inception. The National PARAM Supercomputing Facility was setup in 1998 at C-DAC, Pune with a mandate to offer state-of-the-art High Performance Computing systems and resources to the scientific user community of various academic and research institutes, help them with the know-how and usage of such systems and proliferate HPC awareness in the country.

The supercomputing initiatives PARAM 10000, PARAM Yuva and PARAM Yuva II at National PARAM Supercomputing Facility has contributed to the proliferation of parallel and distribute processing technologies in India which in turn has helped several researchers from various scientific and engineering disciplines to carry out their research more effectively.

PARAM Yuva II

In order to keep abreast with the recent trends in HPC with the accelerator/co-processor technology, an upgrade of PARAM Yuva was planned. This upgraded system called PARAM Yuva II, launched in February 2013 is among the latest addition to the series of prestigious PARAM series of supercomputers built in India. PARAM Yuva II is among the first HPC systems in the country using Intel Xeon Phi along with Intel Xeon for achieving its computing power. With this launch, C-DAC also becomes the first R&D institution in India to cross the 500 TF milestone.

PARAM Yuva

The PARAM Yuva (henceforth referred as PARAM Yuva I), which was built and launched in 2008. It ranked 69^{th} in the Top500 list released in November 2008 at the Supercomputing Conference in Austin, Texas, United States.

PARAM 10000

PARAM 10000 launched in 1998 with 100 GFlops peak performance and set the path for future developments to come.

A typical system would contain 160 CPUs and be capable of 100 GFLOPS but, it was easily scalable to the TFLOP range. Exported to Russia and Singapore.

Technical Affiliation Scheme of NPSF

The users from various Universities, IITs and other R&D institutions have the advantage of the reliability and availability associated with National Knowledge Network for accessing computing resources at NPSF. The scientific community use this computing facility through the Technical Affiliate Scheme of NPSF, C-DAC. Under this, the Chief Investigator (Faculty/Scientist at University/Institute/R&D Lab) enrolls as Technical Affiliate, the researcher along with his/her student(s)/collaborator(s) can get user accounts on NPSF resources and avail computing time for their research work. Prospective users can send their queries to *npsfhelp@cdac.in*.

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1.2 System Insights

Three Subclusters	
Subcluster-1	**PARAM Yuva II:** 221 nodes cluster of Intel server system R2000GZ with Dual socket Intel Xeon E5 2670 (Sandy Bridge) Processor per node Eight CPU cores per socket, 2.6 GHz Two Intel Xeon Phi 5110P per node Infiniband FDR interconnect Partitions: TESTp, FDRp, BIGJOBp, SDSp
Subcluster-2	60+ nodes cluster of HP Proliant DL580 G5 with Quad socket Intel Xeon X7350 Processor per node Four CPU cores per socket, 2.93 GHz System interconnects: PARAMNet3, Infiniband DDR Partition: DDRp
Subcluster-3	Four nodes cluster of Supermicro SuperServer 1027GR-TRF with Dual socket Intel Xeon E5 2650 (Sandy Bridge) Processor per node Eight CPU cores per socket, 2.6 GHz Two NVIDIA GPU Tesla M2090 per node Infiniband FDR interconnect Partition: GPUp
Storage	PFS based scratch space with 10 GB/s write bandwidth User Home Area: 197TB Archival: 800TB

Software

Operating System: CentOS v6.2, Kernel v2.6.32-220

Intel Cluster Studio XE 2013

Intel Cluster Studio XE 2015

PGI Cluster Development Kit

Applications

Libraries and software for file formats, data bases and math

Many scientific applications for material science/quantum chemistry, molecular modelling, computational fluid dynamics, climate modelling, circuit simulations and many more like aerospace engineering.

1.3 Highlights

1. NPSF HPC services were briefly interrupted due to failure in storage subsystem from 5^{th} May, 2018, 1100 Hrs to 5^{th} May, 2018, 1645 Hrs. Emergency maintenance was carried out to correct the fault and lasted around 3 hours 45 minutes, after which services were restored and system made online for job execution.

2. Apart from NPSF operations, team members are faculty of Advanced Computing Training School (ACTS), C-DAC for PG Diploma course titled "HPC System Administration (HPC-SA)". The diploma course is of 6 month duration with two batches in a year. As a faculty, delivering lectures, oversee and guiding during lab practice, conduction of end module lab exams are some of the obligations met.

3. As part of C-DAC's tradition, NPSF team participated to showcase NPSF during National Science Day celebration at C-DAC, Pune, which fell on February 28, 2019. PARAM Yuva II model display attracted most attention by school students and general public alike. In total, around 1700 visitors (Students from various colleges/institutions and schools) from Pune and nearby districts of Mumbai, enjoyed the interactive technical sessions and visit to NPSF.

4. Lectures and talks by NPSF team

   - **Ms. Nisha Agrawal** mentored IIT Dharwad team at GPU Application Hackathon 2018 (GAH-2018), a hackathon event to investigate and implement latest parallelization and optimization techniques for upscaling scientific application on GPGPUs. This event was jointly organized by openACC.org, NVIDIA, C-DAC and IISER, Pune during 17th to 21st September, 2018
   - **Mr. Pankaj Dorlikar** delivered lecture and conducted hands-on session on topic "Anatomy of a job in HPC facility & Related Aspects" during 7 days workshop on HPC at NIT, Kurukshetra. - September 17-24, 2018
   - **Ms. Nisha Agrawal** delivered lecture and conducted hands-on session on topic "Introduction to GPU and Cuda Programming" during 7 days workshop on HPC at NIT, Kurukshetra. - September 17-24, 2018
   - **Ms. Nisha Agrawal** was invited as an expert to conduct session on "MPI & CUDA" for faculties and students of Pune Institute of Computer Technology (PICT), Pune. - September 29, 2018
   - **Ms. Nisha Agrawal** delivered invited talk on "MPI Programming" for faculties and students of Pune Institute of Computer Technology (PICT), Pune. - February 16, 2018

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1.4 NPSF in Last Six Years

Below are some of the NPSF statistics of last six years i.e Year 2013-18.

The statistics includes variation in cluster utilization, year-wise total number of projects, number of Ph.Ds & publications produced using NPSF.

1. **3,69,490** Jobs completed processing.
2. **1131** Users.
3. **114** Institutions.
4. **302** Projects.
5. **49** Completed Ph.Ds.
6. **322** Publications.
7. **252** Total Ph.D. Students.

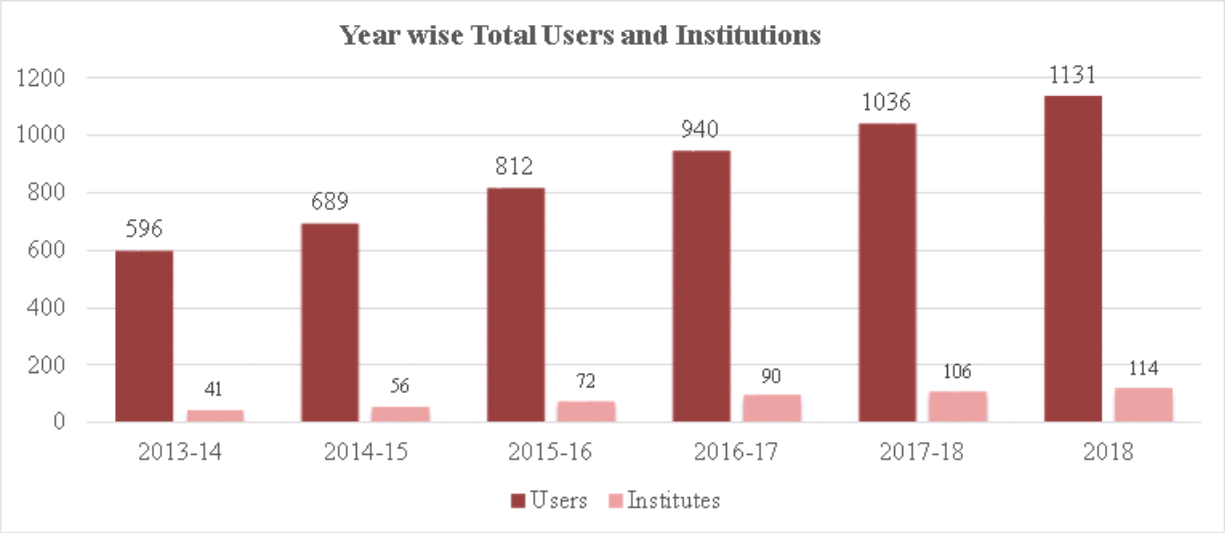


Table: Year wise total users and institutions

Year	Users	Institutes
2013-14	596	41
2014-15	689	56
2015-16	812	72
2016-17	940	90
2017-18	1036	106
2018	1131	114

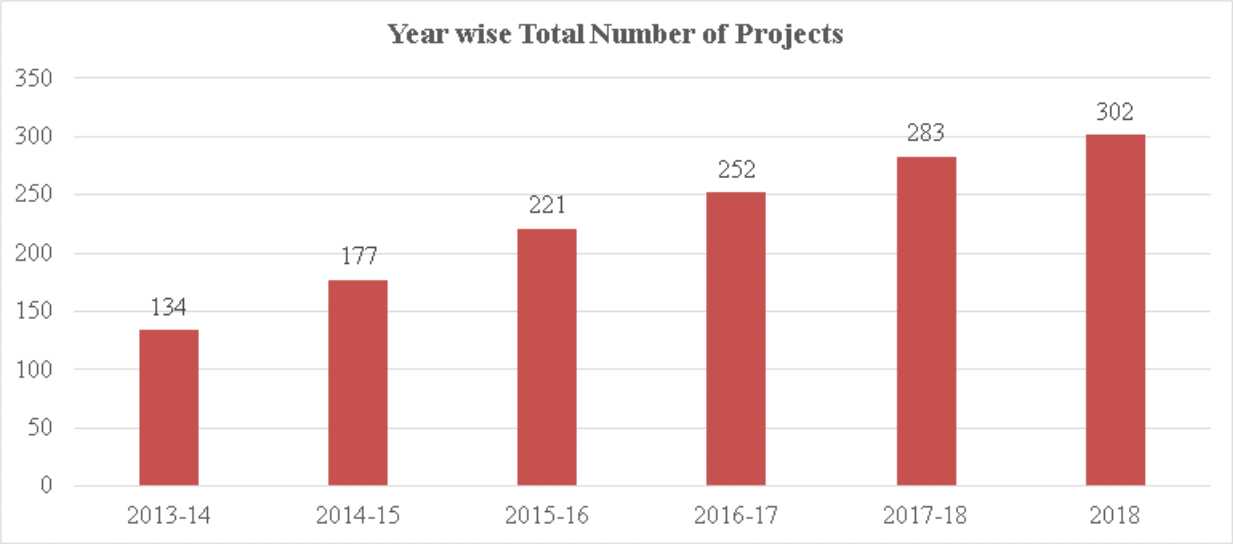


Table: Year wise total number of projects

Year	Number of Projects
2013-14	134
2014-15	177
2015-16	221
2016-17	252
2017-18	283
2018	302

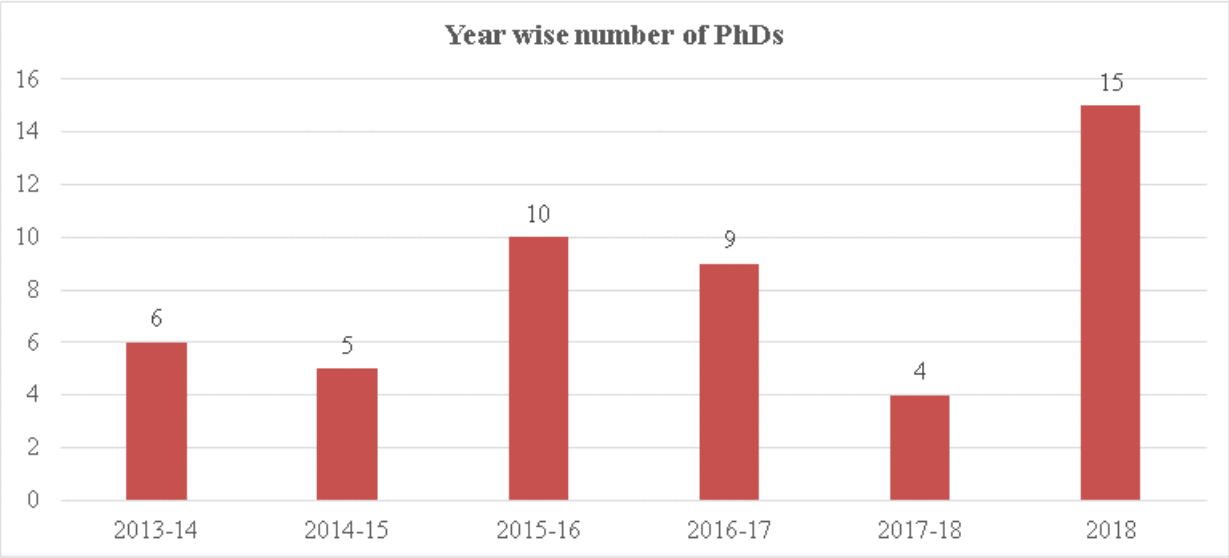


Table: Year wise number of PhDs

Year	Number of PhDs
2013-14	6
2014-15	5
2015-16	10
2016-17	9
2017-18	4
2018	15

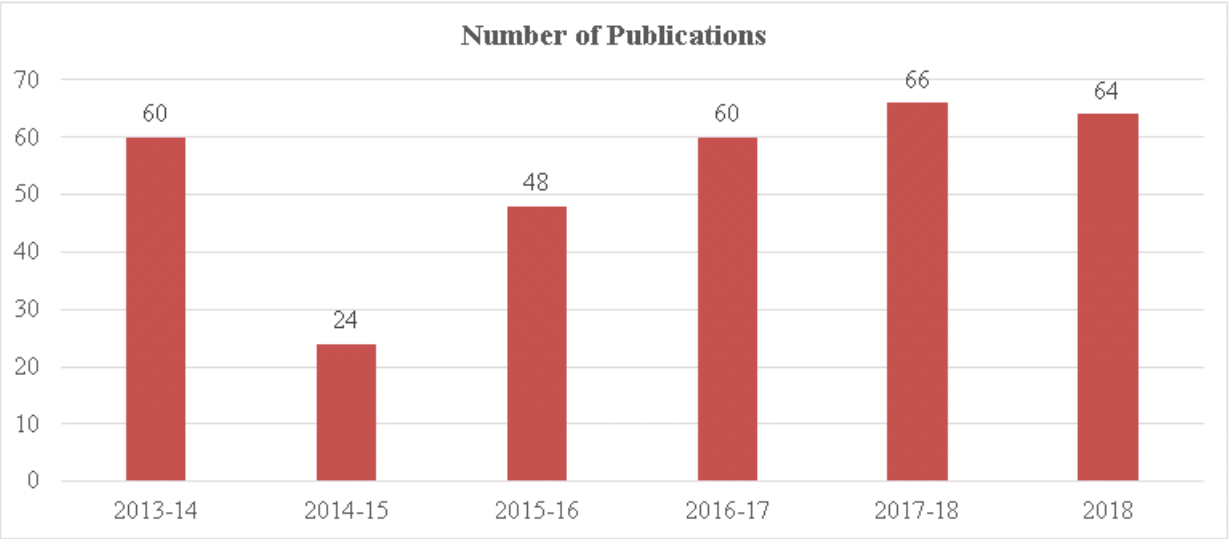


Table: Year wise number of publications

Year	Number of Publications
2013-14	60
2014-15	24
2015-16	48
2016-17	60
2017-18	66
2018	64

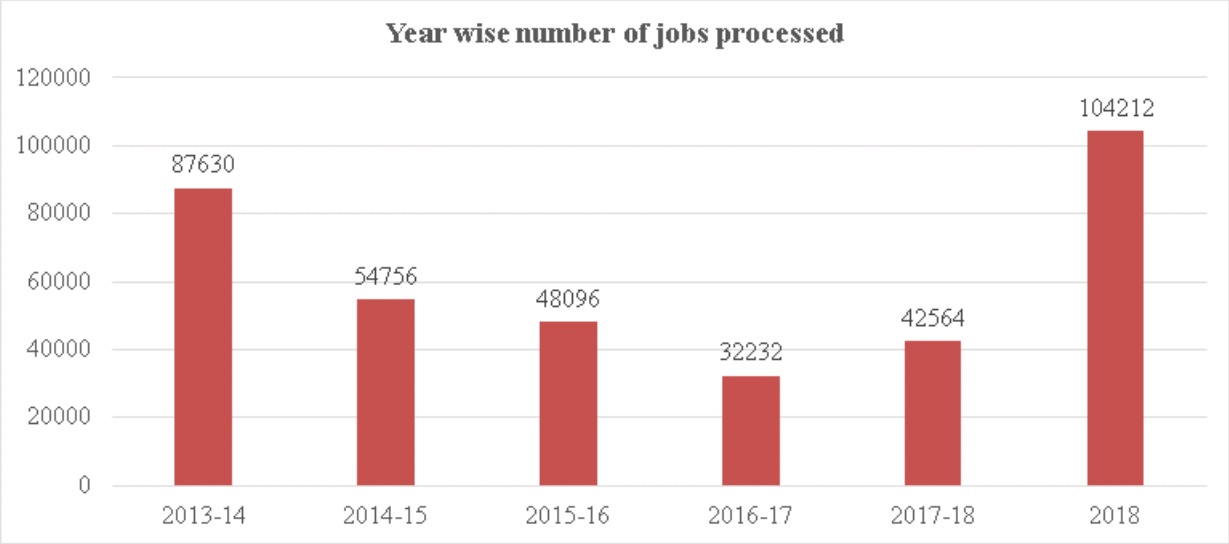


Table: Year wise number of jobs processed

Year	Number of jobs processed
2013-14	87630
2014-15	54756
2015-16	48096
2016-17	32232
2017-18	42564
2018	104212

Table: Year wise number of support calls

Year	Number of support Calls
2013-14	502
2014-15	1482
2015-16	1337
2016-17	1135
2017-18	1137
2018	1121

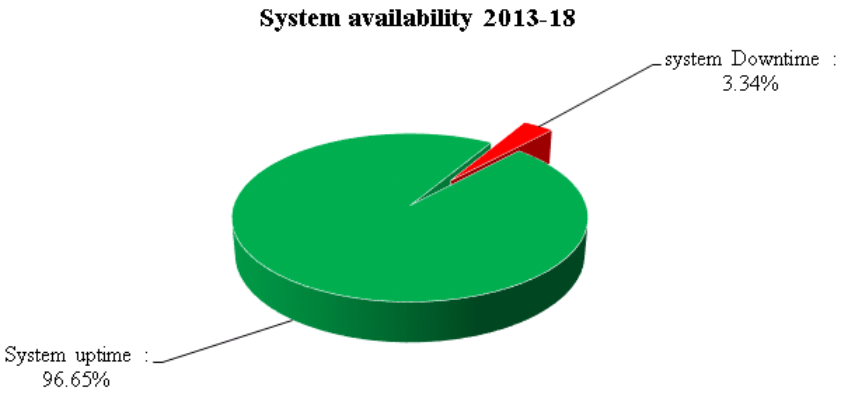
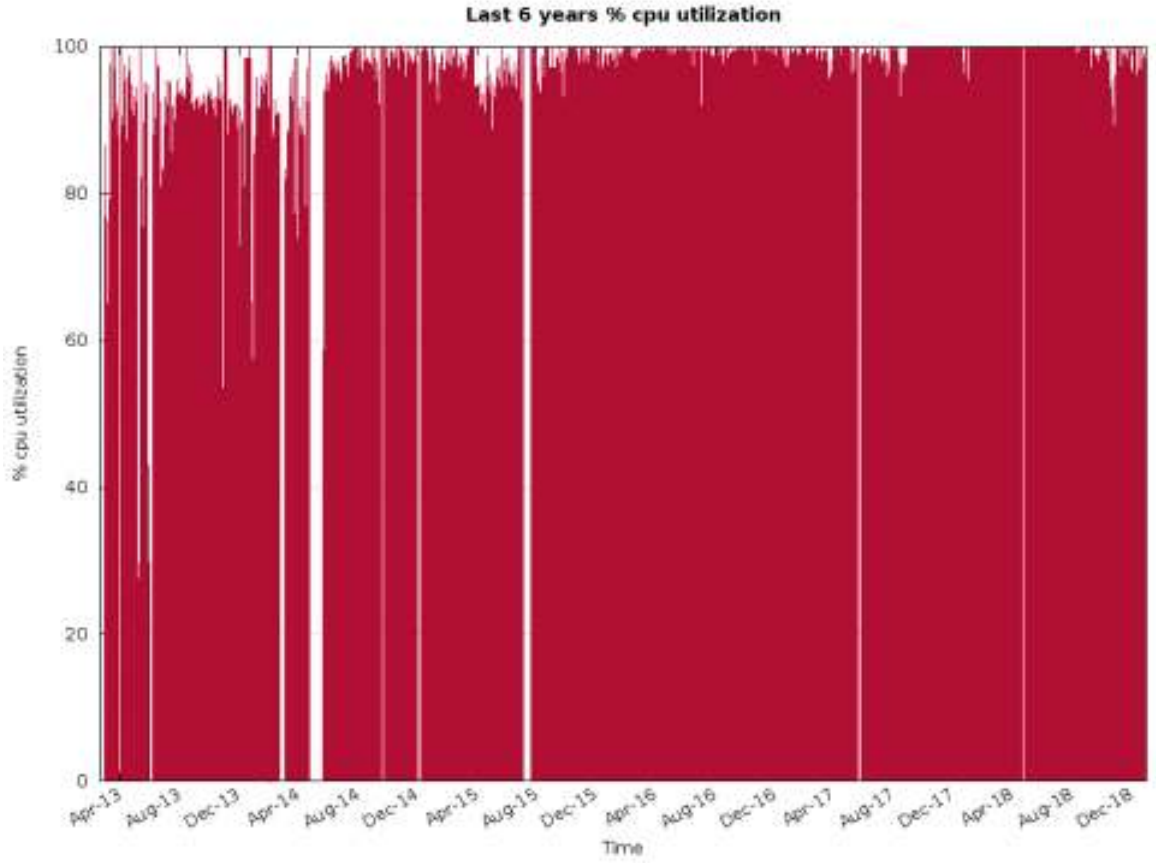


Table: System availability

Year	Uptime(%)	Downtime(%)
2013-14	93	7
2014-15	91.6	8.36
2015-16	97	3
2016-17	99.2	0.8
2017-18	99.17	0.83
2018	99.95	0.05



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2

Users Views

Quotes are extracted from e-mail communications, work reports submitted and publications notified.

2.1 Feedbacks

"PARAM Yuva II has helped me immensely in guiding my Ph.D. students and my Postdoc on a wide range of research problems. The helpdesk has responded with great promptitude in installing different programs modules required by us from time to time. In short, helpdesk has been remarkably supportive. We owe the deepest debt of gratitude to CDAC-Pune and the support team of PARAM Yuva II.

CDAC, Pune has been doing a wonderful job for many years in helping Computational Scientists across India in their active pursuit of research. The strong computational support provided by CDAC-Pune enables us to pursue good quality research. I would like to appeal to the Govt. of India to allocate substantial funds to CDAC-Pune to support the latter in their future endeavors, which includes upgrading their HPC systems. Any HPC system gets outdated in five years. Moreover, the usage of Param Yuva II is really high. Param Yuva II caters to users from all over India. CDAC-Pune is in dire need of a strong funding support from the Govt. of India. Integration of the latest computational resources into the current HPC system is the crying need of the hour. "

Dr. Abir De Sarkar, Scientist-E/Assoc. Prof. & Dean (Academics), Institute of Nano Science and Technology (Autonomous Institute supported by the Departmentof Science and Technology,Government of India), Mohali

"As the computing facility at NPSF is efficient, robust and extremely reliable, the complex computations required for our projects have been executed successfully without any hindrance. This is because of the proper maintenance of Yuva-II cluster by the NPSF team. Furthermore, the assistance provided by the NPSF team for installation of computational packages is also extremely appreciable.
NPSF team has always been very helpful and efficient. If asked for help regarding any simulation package or some difficulties related to the cluster, they are always very prompt in replying and keen on following-up on the problem. This efficiency of NPSF team needs to be highly acknowledged as it helps to keep the projects unaffected due to technical and computational difficulties. "

Dr. Ankita Katre (DST-INSPIRE Faculty), Centre for Modeling and Simulation, S P Pune University, Pune

"I could able to do progress in my Research Project and NPSF support help to complete my calculations using parallel run. "

Dr. Anurag Prakash Sunda,
Central University of Rajasthan

"Our experience of using NPSF is great. Due to NPSF, we are able to do expensive calculations in a very short time. We wish to thank National NPSF for providing the computation facility by PARAM Yuva II cluster.

It is very difficult to carry out some phonon calculations because the given wall time (maximum 7 days) is not sufficient. We request you to give some extra time to counter these type of expensive calculations. "

Dr. Anver Aziz (Assistant Professor),
Jamia Millia Islamia, New Delhi

"The computational facility provided by CDAC is of great support to the Ph.D. students and M.Sc. students to pursue their research projects and timely completion of research work. The benefit of the NPSF is that the simulations can be completed in short time. The NPSF facility is easy to access and the staff at CDAC is very cooperative and quickly response to our queries. We thank the entire team of NPSF for their extended support and cooperation. "

Deepti Goyal (Ph.D.), Assistant Professor,
Sri Guru Granth Sahib World University, Fatehgarh Sahib, Punjab

"It's a nice experience of using NPSF, quick response of querries and helping towards installations. "

Dr. Jagdish Kumar,
Central University of Himachal Pradesh

"For the successful compilation of my project I could finish some important jobs using NPSF facilities which was possible because of good technical support from C-DAC team.

CDAC, Pune has been doing a wonderful job for many years in helping Computational Scientists in their active pursuit of research, across India. The strong computational support provided by CDAC-Pune enables us to pursue good quality research. The numbers of nodes are not enough to run the calculation in less queue time therefore. I would like to draw attention of Indian Government to provide enough financial support to NPSF-C-DAC so that the latest Computational facilities can be provided to users by C-DAC. "

Dr. K.C. Bhamu,
CSIR-NCL, Pune

"We could handle millions of dsRNA sequences against thousands of human transcriptome sequences in a very shorter period of 2 months. We thank NPSF for allowing such a facility for us. "

K. Jeyaram, Scientist-D,
Institute of Bioresources and Sustainable Development (IBSD)

"As mentioned above, our simulations are memory and processor intensive which we could smoothly carry out in the NPSF facility. Many different compilers are available in the facility

and we could select the right compiler for our codes. We definitely look forward to using the facility continuously "

Dr. Manikandan Paranjothy, Assistant Professor,
Indian Institute of Technology Jodhpur

"The work involved under our project requires heavy computational resources. On ordinary machines or servers, this type of work cant be possible. We are fortunate to have C-DACs NPS facility which enabled us to perform complex computational work involving Density Functional Theory (DFT) calculations. We have sometimes utilized more than 100 cores to perform the calculations of hybrid halide perovskite materials and these calculations were completely in efficient time frame always. Without NPSF facility, the theoretical research involving heavy computation can never to thought. The queuing system to fire the job is wonderful, it gives the equal chance for every user to submit their job. The NPSF staff members are very helpful and cordial. They helped us time to time in writing the script and installation of some software in our account. We are thankful to supporting staff of NPSF for making all the computational work possible for us. "

Dr. Manish K. Kashyap,
Kurukshetra University, Kurukshetra

"NPSF technology provide easy access and helped us for scientific application to carry out our research work. "

Dr. Mrs. M. D. Deshpande, Professor,
H. P. T. Arts & R. Y. K. science, College, Nasik

"The computing resources provided by NPSF is indeed a great help to us as it mostly fulfils our growing needs of the computing resources to pursue world class research activity without developing any local HPC. This is indeed a great initiative by Govt. of India to provide resource to the researcher of relatively smaller institute that the lack of appropriate man power to manage a data center and generate such huge scale of computing resources. I must appreciate help from NPSF experts and various supporting staffs. They are always easy to approach and quick to resolve the issues related to all issues. "

Dr. Md. Ehesan Ali, Scientist-E,
Institute of Nano Sciences and Technology

"The purpose of NPSF for the contribution of parallel and distribute processing technologies in India which in turn helped for us for the scientific applications to carry out research more effectively. "

Dr. Mrs. M. D. Deshpande, Professor,
H. P. T. Arts & R. Y. K. science, College, Nasik

"We are very much greatfull to the NPSF team for providing the computational resource in support of our project and the technical helps we got it is highly appreciated. "

Dr. Neelanjana Sengupta, Assistant Professor,
Indian Institute of Science Education and Research Kolkata

"I have used NPSF super-computing facility for parallel computations. "

Dr Pankaj Biswas, Assistant Professor,
NIT Silchar, Assam, INDIA

"The NPSF is the most well maintained resource in India. The team was always there to accommodate our querries with quick responses. We have been helped a lot during installations etc. The resource has lead to reduction in our time consumption for carrying these heavy computations. "

Prof. P. K. Ahluwalia,
Physics Department, H. P. University, Shimla (H.P.)

"Access to Param Yuva made these heavy calculations possible. I would also like to thank the staff for the excellent maintenance of the cluster (with minimal amount of downtime) and their prompt help to my students whenever they had any difficulties.

I think one needs to optimize the waiting time for a moderately sized job to start. Presently one needs to wait for days. "

Prasenjit Ghosh, Associate Professor,
Indian Institute of Science Education and Research, Pune

"Performing molecular dynamics simulations is a computationally expensive task. Execution of each of the work described above on a single processor or on a desktop machine takes several days. Using the NPSF computing facility, we have been able to reduce our run-time to a few hours to a few days, depending on the problem. The reduction in time has helped us in speeding up the work significantly. However, these days Param Yuva cluster has a long queue, and as a consequence some of the simple tasks take a long time to start running. Queuing of tasks can be

further streamlined so that separate jobs using single-processors can get queued quickly. "

Dr. Puneet Kumar Patra, Assistant Professor,
Department of Civil Engineering, Indian Institute of Technology Kharagpur

"Benefits: Because of massive computation one can choose the problem without taking too much concern of the massiveness of problem. We do not need to worry about the installation problem thanks to NPSF help service. Experience: We feel delighted and obliged to NPSF for maintaining such a standard of work ethics. We feel a debt of gratitude for the services and try our best to meet NPSF team expectations. "

Raman Sharma (Professor),
Himachal Pradesh University

"The proposed work is one of the important directions both in the fundamental and applied sciences. In addition, the outcome will be beneficial for the research students participating in the projects giving them opportunity to perform scientific investigation at national/international level and to meet and discuss with scientist and students from other international laboratory. This supercomputing collaboration can also be extended for the future. It is expected that the studies performed will lead to publications in refereed international journals and will be suitable for presentation at local and international conferences.

Computational facilities from the Center for Development of Advance Computing (C-DAC) Pune are also gratefully acknowledged "

Dr Sanjeev Kumar Gupta, Assistant Professor ,
St. Xaviers College, Ahmedabad, Gujarat

"3D inversion of Magnetotelluric data is computationally very intensive. Using NPSF significantly reduced the inversion time. Before concluding to a final model one is required to test many

parameters and running the inversion a number of times which is also very much time consuming. We had a very pleasant experience using NPSF where we were given enough of memory as well as in most if the cases the queue time was not very large. And the support which we got over the years were very good. The support staffs always helped and they were very soft. "

Prof. Shalivahan (Dean R&D),
Indian Institute of Technology (ISM), Dhanbad

"1. Param Yuva II has so far been extremely useful for running high resolution (5123 and above) of MHD turbulence using up to 1024 cores. We hope that the waiting time in the queue for these demanding simulations can be further shortened.

2. It has been observed that jobs keep crashing due to node issues severely impacting the smooth running of jobs and causing a delay in timely execution of runs. Although such unforced errors may happen, it will only help the end user if efforts are taken promptly to address and minimize such issues from occurring. In such an event, the user who job failed due to node issues could be allowed to run his/her job on a priority basis to make up for the lost time.

3. For 2D runs, we tested our code successfully on Param Yuva. Scaling this to 3D will require us to use Param Yuva more frequently for cores 2048. In the testing phase the queueing time has improved over last year but is still quite long. However for high cadence output (due to sampling Nyquist criteria), the data transfer to our local computers for analysis is still a problem because of transfer speeds and unavailability of scratch space on Param. We think these issues decreasing the efficiency of the work being carried out. "

Sharanya Sur, Reader Piyali ChaHerjee, Reader (Co-Investigator),
Indian Institution of Astrophysics, Bangalore

"We started using NPSF facility since July 2018, from that time NPSF system admins are very supportive and encouraging by solving all technical issues. We are happy and want to conduct more advanced MD simulations in order to find out solutions to our scientific questions of interest. "

Dr. S Krishnaveni, Assistant professor,
Department of Studies in Physics, Manasagangotri, University of Mysore

"Thank you for providing the resources. The resources provided by NPSF has been acknowledged in the published article. Some hopefully useful feedback on my experience using the service: The actual available resources were significantly less than what was allocated and availability was extremely unpredictable. It might be better to promise a more realistic number of processor hours. It might be useful to benchmark the resources provided with that in international research institutes. The login procedure was painful. It prevented accessing the files through sftp from Linux browsers. Blocking of server access from outside a limited set of ip addresses meant that we could not submit jobs when traveling or when working from home. Perhaps these can be improved. "

Sreejith G J,
IISER Pune

"To understand the conformational dynamics of biomacromolecules, longer timescale simulation is necessary and NPSF is very much useful in this context. It can be even more beneficial, if queue waiting time can be reduced and more GPU can be inducted. "

Thenmalarchelvi Rathinavelan,
Indian institute of Technology Hyderabad

"Excellent supportive response is obtained from the CDAC help team, and we had several fruitful discussions while compiling all the code which we are using for our calculations. We could get all the information from job submission to the final output, and this system is very helpful. The job status process is very helpful; we could figure out several job terminations without any time delay. Here we sincerely thank the CDAC for this great facility and the good support. Continued support

from the CDAC team is highly appreciated and we look for the same in future with enhanced CPU time as we are working on many other projects also, which might be finished on time with the help of CDAC computing time. "

V. Kanchana, Professor,
IIT Hyderabad

"Our calculations are highly compute intensive and the access to the NPSF computing resource enabled us to perform these simulations which otherwise were not possible with the available in-house computing resources in our department. Every dif- ficulty with the execution of the jobs submitted on NPSF is promptly addressed by the NPSF help desk and system administrator. Our experience with the NPSF is highly satisfactory and we find them always genial and responsive to our queries and job related issues. NPSF has been a great boon for the research work that is being performed in my research group and I hope that it continues to re- main functional and available to university researchers to take up research problems that cannot be otherwise addressed at our infrastructure level. "

Dr. Vaishali Shah, Assistant Professor,
Interdisciplinary School of Scientific Computing, Savitribai Phule Pune University

"It was good experience to use NPSF facility "

Dr. Yogesh Sonvane,
Sardar Vallbhbhai National Institute of Technology

2.2 Appreciations

"We are grateful for the assistance offered by C-DAC towards the project "CFD Analysis of 120 mm. FSAPDS Tank Ammunition" carried out by Centre for Modeling and Simulation, SPPU with DRDO. This project was successfully completed in 2016. The results have been reported to DRDO but cannot be shared in any academic journal. This note can serve as an acknowledgement of the computing support provided by C-DAC to test supersonic compressible ow simulations. "

Mr. Sukratu Barve,
Asst. Prof., S P Pune University, Pune

"I feel so proud to be given this wonderful opportunity to use India's best supercomputing facility. It is simply the best because of the wonderful support you all provide. You all work really hard and the same has been reflected truly in the yearly report 2017-18. It is really very well prepared and beautifully organized too.
May you all prosper and achieve all the success in your lives. I am deeply grateful to the Director Sir for giving me access to this supercomputing facility. I hope you will keep helping researchers like me the same way always.
I have been publishing my research works mostly all alone, and hence I am a bit slow in publishing. But I am working hard and have started learning new packages like DFTBaby and DFTB+, which were installed with lots of effort by the NPSF team, especially Ms. Shraddha.
Wishing you all a very bright future ahead. "

Dr. Siddheshwar Chopra
Asst. Prof. , Amity University, Noida

"I introduce myself as Dr. Tulika Gupta, Assistant Professor in Chemistry department, Faculty of Science, Banaras Hindu University (BHU), Varanasi. I am a computational Chemistry, did PhD from IIT Bombay and post-doc from Germany. During my stay in IIT Bombay, I have been tremendously privileged in my research career harnessing your pertinent supercomputing facility.....

Dr. Tulika Gupta,
Assist. Prof. IIT, BHU

"Happy to inform that HPC-SEA group paper, Title: Application of Moderate Resolution Imaging Spectroradiometer (MODIS) Aerosol Optical Depth (AOD) and Weather Research Forecasting (WRF) model meteorological data for assessment of fine particulate matter (PM2.5) over India authored by Mr. Yogesh Sathe, Dr. Santosh Kulkarni, myself and Mr. Sahidul Islam along with NASA USA and CPCB India has been accepted in Scientific journal -Atmospheric Pollution research
The research work is in collaboration with prestigious institute NASA USA and we look forward to many more research activities with them
The modeling simulations were carried out on PARAM Yuva System. We acknowledge NPSF support. "

Ms. Akshara Kaginalkar
Senior Director and HoD, HPC-S&EA
C-DAC, Pune

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2.3 Acknowledgements

"Authors are grateful to Professor Shridhar R. Gadre for making us available his computational facility. Authors are also thankful to Prof. M. V. Waykole, Bhusawal Arts Science and P. O. Nahata Commerce College, Bhusawal for support to this work. Authors are also grateful to C-DAC, Pune for the computational Support."

Dr. Sachin D. Yeole ,
Bhusawal Arts Science and Commerce College, Jalgaon

"Computational resources have been provided by the Centre for Development of Advanced Computing (C-DAC), Pune. Funding for this project has been provided by the Department of Science and Technology, India (Reference : SB/S3/CE/054/2014)."

Prof. Jhumpa Adhikari,
IIT Bombay

"We thank the anonymous referee for a very careful reading of our manuscript that has led to a marked improvement in the clarity of this paper. M.B.K. is grateful to the University of Sheffield and the Hungarian Academy of Sciences for the support received. M.B.K. also acknowledges the open research program of CAS Key Laboratory of Solar Activity, National Astronomical Observatories, No. KLSA201610. P.C. thanks the University of Sheffield for hospitality and support for a visit during which this work was initiated and the CAS PIFI project 2017VMC0002 and National Astronomical Observatories, Beijing, for support. The simulation was carried out on NASAPleiades supercomputer under GID s1061. P.C. also acknowledges computing time awarded on the PARAM Yuva-II supercomputer at C-DAC, India, under the grant name Hydromagnetic-Turbulence-PR. We have used the 3D visualization software Paraview for volume rendering and field line plotting. R.E. is grateful to the Science and Technology Facilities Council (STFC; grant Nos. ST/ L006316/1 and ST/M000826/1) UK and the Royal Society for their support. The authors also express their gratitude to Christopher J. Nelson and Michael S. Ruderman (both at 11 The Astrophysical Journal, 857:103 (12pp), 2018 April 20 Kors3s, Chatterjee, & Erd9lyi University of Sheffield, UK) for a number of useful discussions and improving the manuscript."

Dr. Piyali Chatterjee,
IIAP Bangalore

"Mr. S. Penislusshiyan acknowledges Department of Science and Technology, Ministry of Science and Technology, India, for the award of INSPIRE fellowship [Ref.No. IF140651] to carry out this research successfully. Ms. L. Chitra acknowledges Science and Engineering Research Board, India for the award of National Post-Doctoral Fellowship (Ref. No. PDF/2015/000252). The authors thank the C-DAC Garuda, Bangalore for providing the supercomputing facility."

Prof. P. Kumaradhas,
Periyar University, Salem

"VRC thanks the Centre for Development of Advanced Computing, Pune, India for computational resources"

Dr. V. Ravi Chandra,
NISER, Bhubneshwar

"This research was supported in part by the NSF Astronomy and Astrophysics Grants Program (grant 1615100) and the University of Colorado through its support of the George Ellery Hale visiting faculty appointment. We acknowledge the allocation of computing resources provided by the Swedish National Allocations Committee at the Center for Parallel Computers at the Royal Institute of Technology in Stockholm. This work utilized the Janus supercomputer,

which is supported by the National Science Foundation (award number CNS-0821794), the University of Colorado Boulder, the University of Colorado Denver, and the National Center for Atmospheric Research. The Janus supercomputer is operated by the University of Colorado Boulder. The input files as well as some of the output files of the simulation are available under http://www.nordita.org/∼brandenb/projects/ spherical-geom. PC acknowledges computing time awarded on the PARAM Yuva-II supercomputer at C-DAC India under the grant name Hydromagnetic-Turbulence-PR."

Dr. Piyali Chatterjee,
IIAP Bangalore

"YP thank the C-DAC NPSF PARAM YUVA-II supercomputing facility, Pune, India, for providing the required computational resources. YP and KS also thank the LRZ: Leibniz Supercomputing Centre, Munich, Germany, for providing computational resources as part of the 4th SFB TRR40 Summer Program 2017 held at TUM, Germany. JL is supported by the National Science Foundation (Grant CBET-1453633) and the Air Force Office of Scientific Research (Grant FA95501610385). Preliminary results of this article were presented at the0Tenth International Symposium on Turbulence and Shear Flow Phenomena (TSFP10), Chicago, IL, USA, July 69, 2017."

Mr. Yogesh Prasad,
IITB

"We acknowledge the Indian Meteorological Department for providing daily gridded rainfall data. We also thank PARAM Yuva supercomputer of National PARAM Supercomputing Facility at the Centre for Development of Advanced Computing (CDAC), Pune for the computational support. NCEP reanalysis, MODIS and radiosonde datasets are obtained from the we-bresources0`http://www.cdc.noaa.gov/`*,*`http://dss.ucar.edu/datasets/ds083.2/data/`*,0*`http://disc.sci.gsfc.nasa.gov/giovanni`*, and 0*`http://weather.uwyo.edu/upperair/sounding.html`*, respectively. We acknowledge use of the WRF-Chem preprocessor tools provided by the Atmospheric Chemistry Observations and Modeling Lab (ACOM) of NCAR."*

Ms. Akshara Kaginalkar,
C-DAC, Pune

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Dr. Mukul Kabir ,
IISER, Pune

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Dr. Anurag Srivastava,
IIITM , Gwalior

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A. C. Vutha for fruitful discussions. Computations were carried out on the Tokyo Tech Computer Cluster (CHIYO), Tokyo, Japan, Inter-University Accelerator Centre, New Delhi, India, and National PARAM Supercomputing Facility, C-DAC, Pune, India"

Dr. B.P. Das ,
IIAP Bangalore

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Dr. D. R. Roy,
SVNIT, Surat

"Author want to thanks to Vishwakarma Institute, Craidlr Technology and CDAC Pune for allowing to carry out this study. Also, author want to thanks all others for direct and indirect help."

Dr. Vikas Kumar,
C-DAC Pune

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3

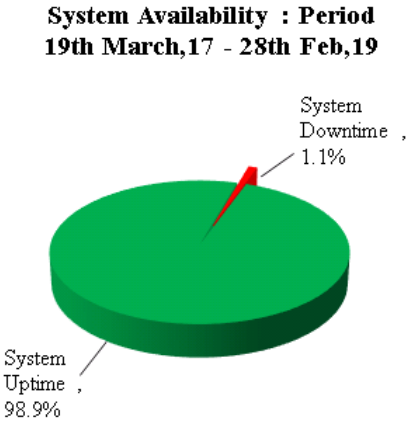
Statistics

In Year 2018 : Users added : 103 ; Institution added : 14 ; Jobs processed : 104212

3.1 System

System availability

System availability is indicator of the healthy and operational system. With only maintained. It can be seen that as compared to last year, the uptime of the system has increased to 99.95% from 98.9%.



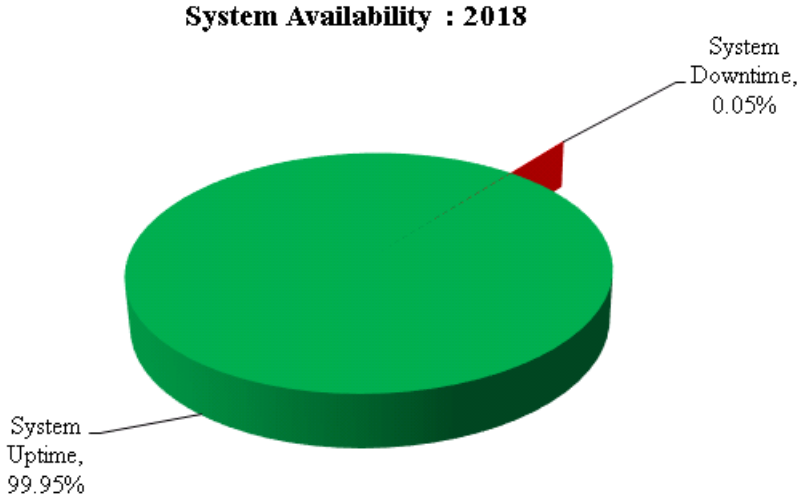
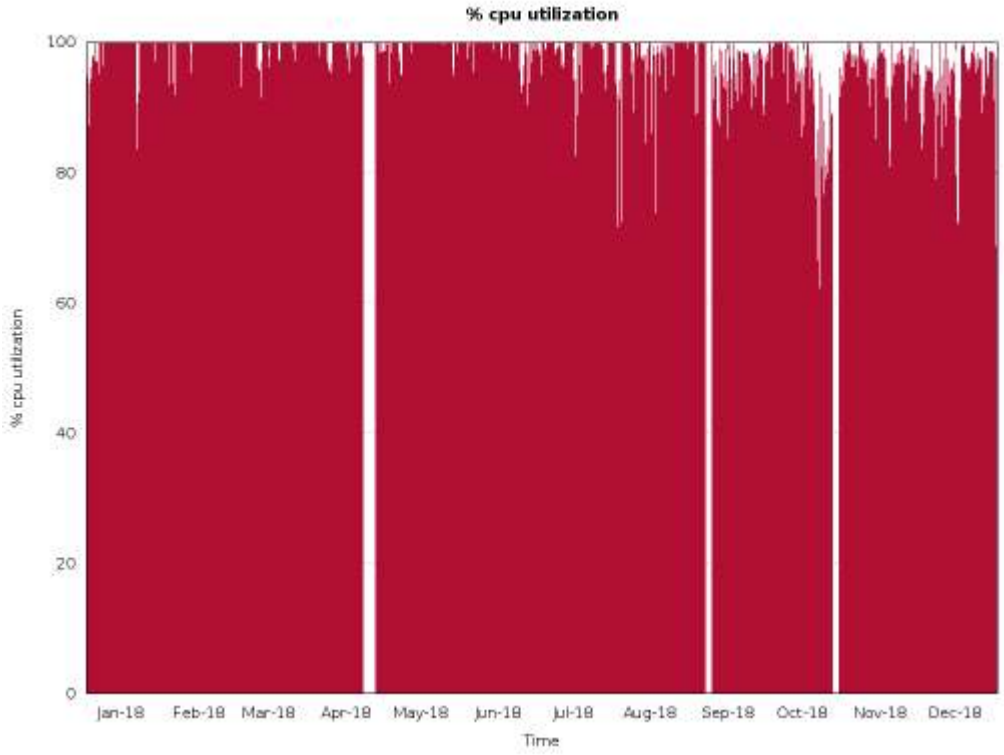


Table: System availability

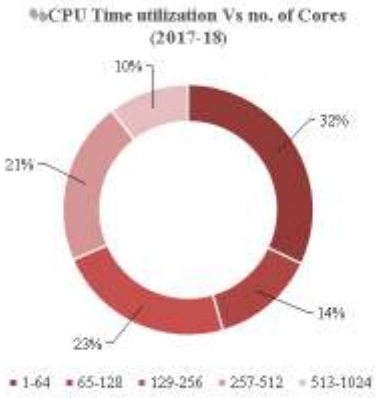
Duration	Total Time	Downtime
16Mar'17-28Feb'18	350 Days(total : 8400 Hours)	3 Days, 21 Hours (total : 93Hours)
1Jan'18-31Dec'18	365 Days(total : 8760 Hours)	5 Hours, 13 Minutes

System utilization

System utilization (% cpu utilization) is calculated as % of cpu cores used by the batch jobs for computation, out of total available number of cpu cores, as recorded by the scheduler at regular intervals. It can be seen that the System utilization has most of the times remained above 90% throughout the year.



CPU time utilization w.r.t. job sizes



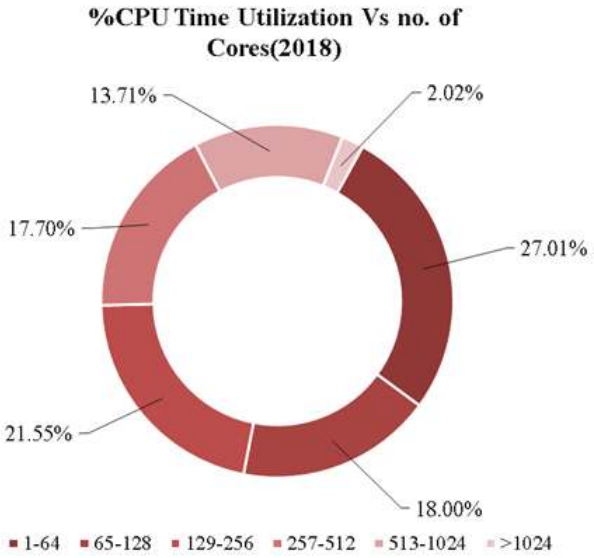
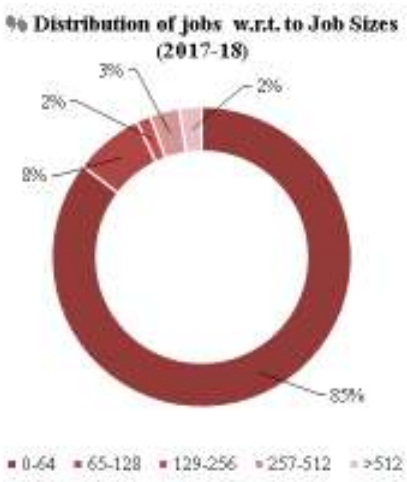


Table: CPU time utilization w.r.t. job sizes

	CPU time utilized (in seconds)	
Job Sizes	**2017-18**	**2018**
1-64	37931720605	38430639920
65-128	15937841856	25613338018
129-256	27205492336	30660088882
257-512	24952112240	25185869864
513-1024	12348922448	19504730320
>1024	0	2872174464

Above doughnut indicates % distribution of cpu time among different job sizes (binning of number of cores). It can be seen that there is 5% increase in use of cputime by big jobs (jobs requiring more than 64 cores). Also, there is new entrant in the job sizes which is jobs requiring more than 1024 cores and it has consumed 2% of the total cpu time is consumed by big jobs. This is also indication of increase in % of capability computing.

% Distribution of jobs w.r.t. job sizes



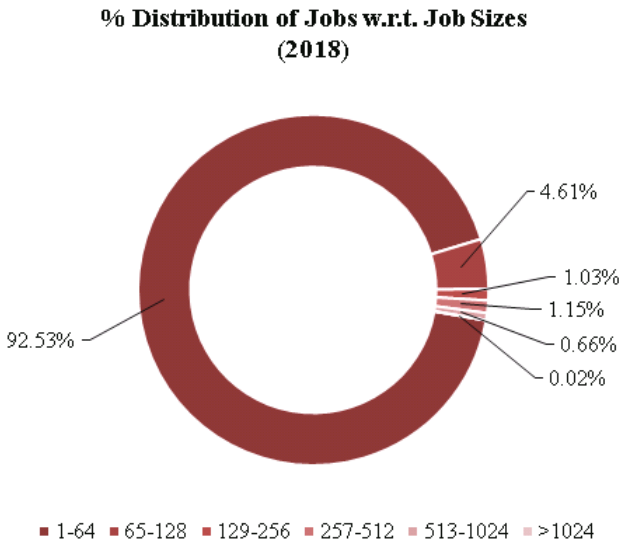


Table: Distribution of jobs w.r.t. job sizes

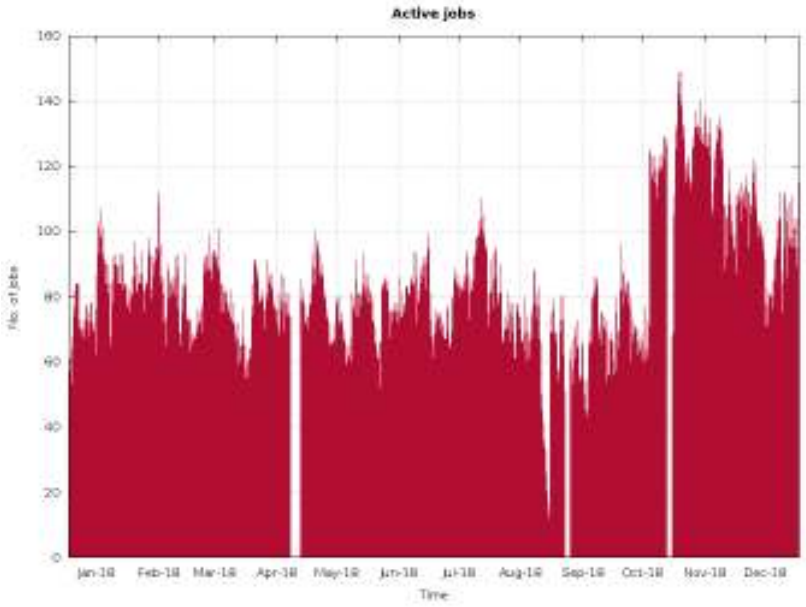
	Job Count	
Job Sizes	**2017-18**	**2018**
1-64	36345	96430
65-128	3181	4807
129-256	663	1077
257-512	1366	1197
513-1024	1009	684
>1024	0	17

Above doughnut indicates % distribution of number of batch jobs binned by number of cores. The % of number of big jobs (jobs requiring more than 64 cores) is decreased by 7.5% however, the percentage of cputime consumed by the big jobs is 5% more than the percentage of cputime consumed by the big jobs last year.

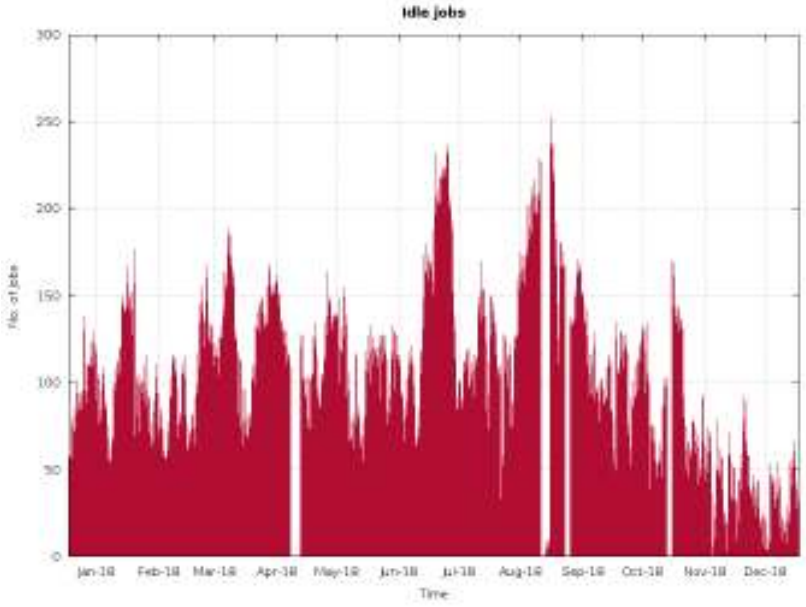
Active jobs, idle jobs & system backlog

A job on NPSF HPC system is a construct comprising of parallel program, resource requirements in terms of memory & CPU cores and indicative time for which these resources are required for successful completion. The two plots below presents figures for 1) Active jobs currently being processed, & 2) Idle jobs eligible for execution and waiting to be allocated resources

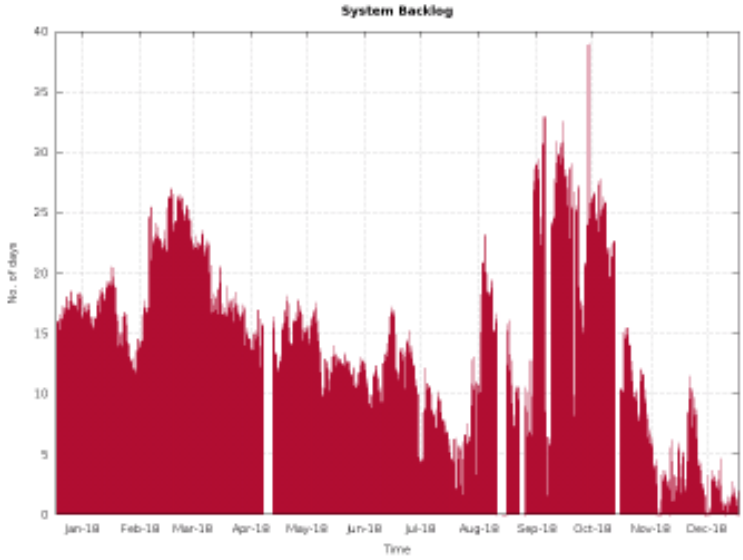
Active jobs



Idle jobs



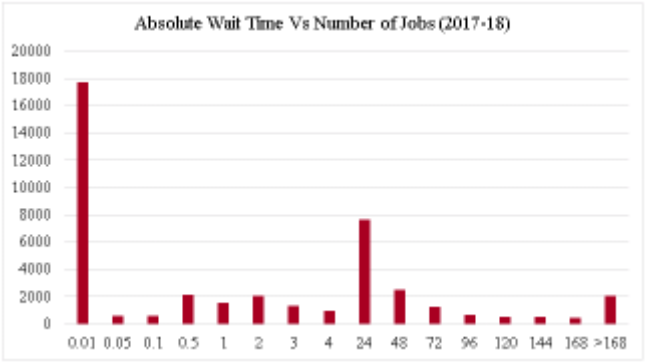
System backlog



System backlog is computed as the total time required to process all idle jobs in the system, given that 1) No new jobs are introduced, & 2) State of the system is not changed, including compute capacity.

Absolute waittime Vs no. of jobs

Absolute waittime for a job is the time spent in the queue, after submission, till allocation of resources and execution.



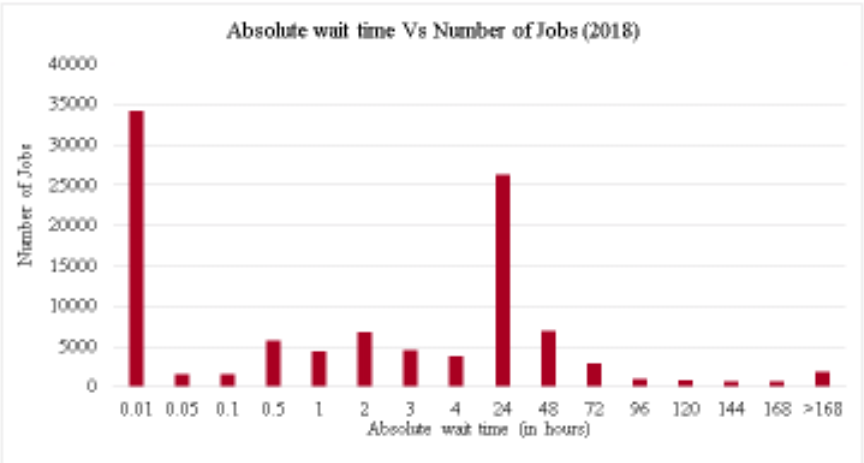


Table: Absolute waittime Vs no. of jobs

	No. of jobs	
Absolute wait time (in hours)	**2017-18**	**2018**
0.01	17730	34243
0.05	622	1641
0.1	580	1528
0.5	2136	5826
1	1538	4348
2	2075	6836
3	1310	4610
4	951	3836
24	7628	26366
48	2518	7017
72	1238	2915
96	702	1051
120	553	823
144	517	722
168	474	642
>168	2038	1942

Above presentation is irrespective of job size. In 2018, As compared to last year, there is 22% decrease in the absolute wait time of the jobs that spend more than one day in the queue waiting for the resources. Also, in 2018, less than 15% of the jobs have spent more than one day in the queue and 32% of the jobs have spent less than or equal to 6 seconds in the queue.

Execution Time Vs Number of Jobs

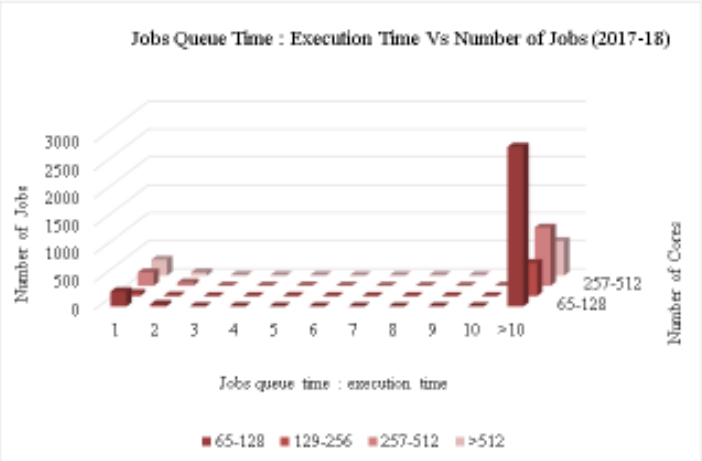
Table: Execution Time Vs Number of Jobs

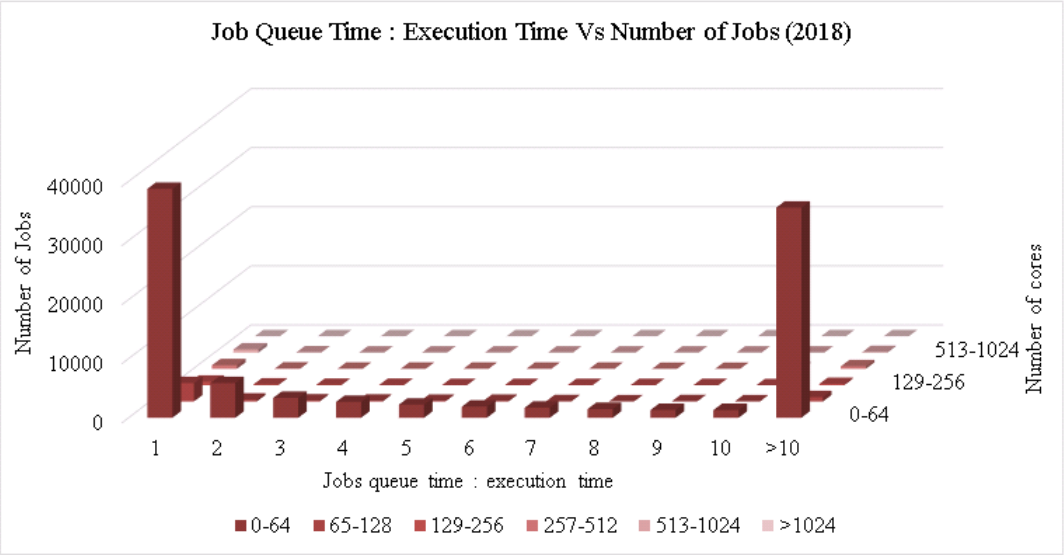
	Number of Jobs	
Execution Time (in hours)	**2017-2018**	**2018**
0.01	9031	26162
0.05	3739	10208
0.1	1848	6328
0.5	5588	20294
1	3035	7435
2	4308	9833
3	3294	6876
4	879	2110
24	5963	8918
48	1504	2167
72	724	1125
96	499	654
120	471	562
144	451	383
168	1229	1017
>168	0	65

Above graph represents execution time of the jobs in hours. It is seen that only 1% of the total jobs executed for 7 days which is the maximum limit of the wall time of the jobs as compared to only 2.9% % of the total jobs executed for 7 days last year.

Relative measure of job wait time with respect to its execution time, binned by job sizes

Below representation is relative measure of job wait time with respect to its execution time, binned by job sizes. X-axis has the ratio of job waittime : execution time, Y-axis is the number of such jobs and on Z-axis, jobs are binned by number of CPU cores.





It can be seen that majority of jobs spends time in waiting, which is >10 times their execution time. Bin sizes for above is 65 CPU cores onwards and statistics for jobs requesting less than that is given below.

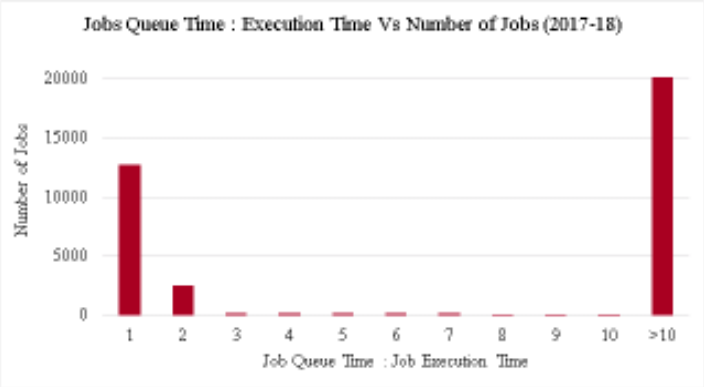
This segregation is made because job count for 1 to 64 CPU cores, being very high, diminishes bars for other job sizes, thus making observable distance between them nondescript.

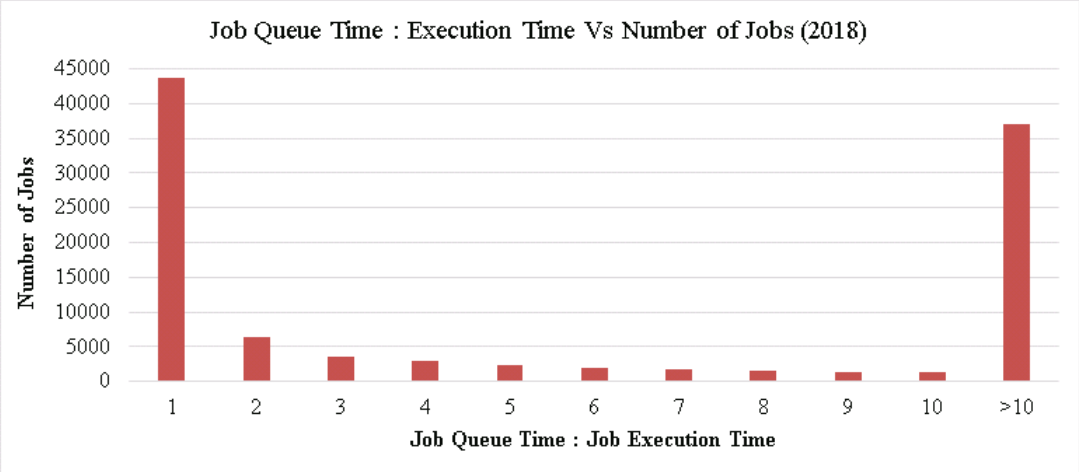
Table : Ratio of job waittime : execution time Vs number of jobs

2017-18	1	2	3	4	5	6	7	8	9	10	>10
1-64	12752	2514	185	158	160	148	137	92	69	35	20123
65-128	270	40	5	5	2	2	2	0	1	4	2861
129-256	54	11	1	1	2	1	1	1	1	0	593
257-512	242	61	3	4	6	3	0	2	0	4	1044
>512	285	56	10	6	6	3	4	8	5	7	619

Table : Ratio of job waittime : execution time Vs number of jobs

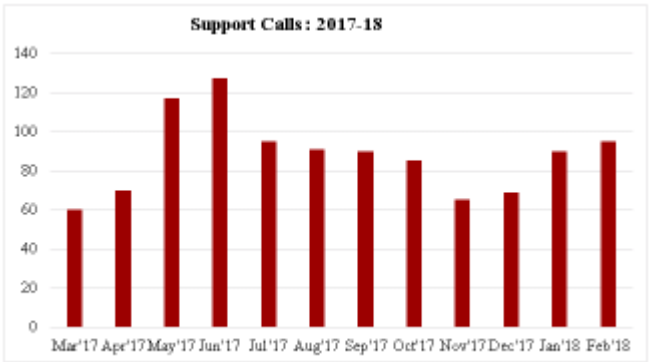
2018	1	2	3	4	5	6	7	8	9	10	>10
0-64	38746	5867	3382	2688	2225	1889	1701	1488	1336	1310	35577
65-128	3107	328	174	124	99	95	62	33	42	32	730
129-256	588	104	66	40	21	13	17	15	9	5	203
257-512	622	48	16	12	17	13	20	4	5	6	436
513-1024	534	27	9	11	9	2	2	4	2	0	84
>1024	15	3	2	2	0	0	0	0	0	0	8





42% of the jobs have spent less than or equal amount of time in the queue as of its execution time (irrespective of job sizes), as compared to 32% of the jobs last year. This is indicator of increased turnaround time of the jobs as compared to last year.

User support calls



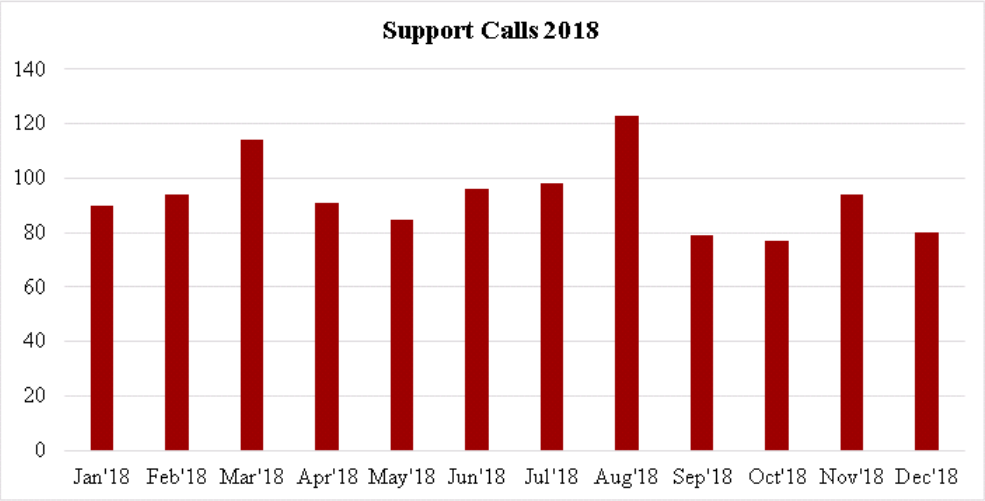


Table : Number of support calls

2017-18	Mar	Apr	May	Jun7	Jul	Aug	Sep	Oct	Nov	Dec	Jan'18	Feb'18
	60	70	117	127	95	91	90	85	65	69	90	94
2018	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
	90	94	114	91	85	96	98	123	79	77	94	80

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State wise CPU time utilization in %

NPSF user community is geographically distributed across 24 out of 36 States and Union Territories. Maharashtra being the highest in utilization of cpu time. This is complemented by the fact that NPSF has has maximum number of users from Maharashtra.

Table: State wise CPU time utilization in %

State or Union Territory	Short Name	% CPU Time
Andhra Pradesh	AP	0
Arunachal Pradesh	AR	0
Assam	AS	0.606798
Bihar	BR	0.000000023
Chandigarh	CH	1.01463
Chattisgarh	CG	0
National Capital Territory of Delhi	DL	0.737428
Goa	GA	0.0537415
Gujarat	GJ	4.17614
Haryana	HR	0.365878
Himachal Pradesh	HP	3.25505
Jammu and Kashmir	J&K	0
Jharkhand	JK	0.103648
Karnataka	KA	9.87101
Kerala	KL	0
Madhya Pradesh	MP	0.44944
Maharashtra	MH	61.5849
Manipur	MN	0.0875128
Meghalaya	ML	0
Mizoram	MZ	0
Nagaland	NL	0
Odisha	OD	0.706773
Puducherry	PY	0.173856
Punjab	PB	9.3999
Rajasthan	RJ	1.45717
Sikkim	SK	0
Tamil Nadu	TN	1.08276
Telangana	TS	2.5288
Tripura	TR	0
Uttar Pradesh	UP	1.51729
Uttarakhand	UK	0.311054
West Bengal	WB	0.516182

CPU Time Utilization in %

;

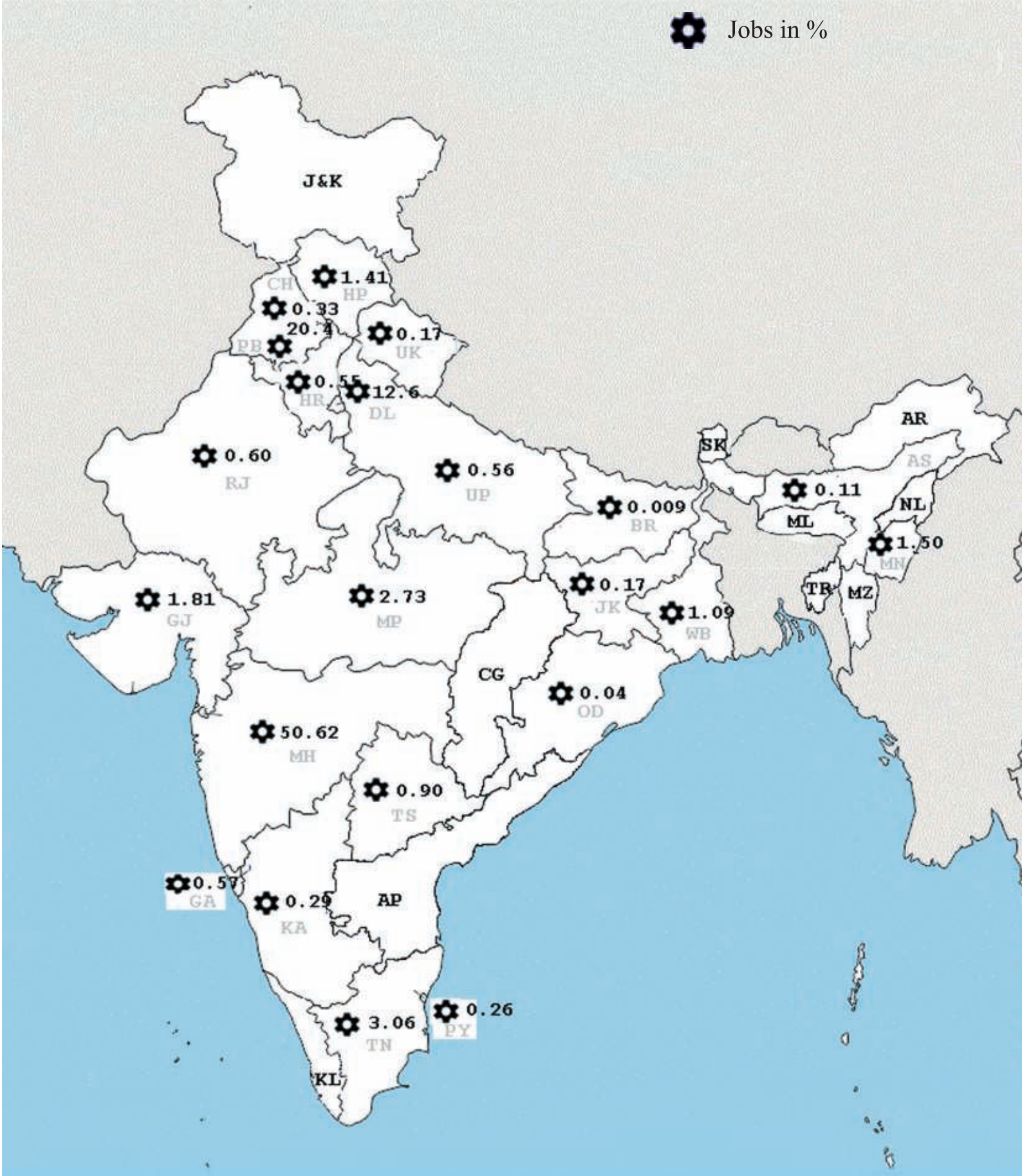
Disclaimer: The map depicted above is only a pictorial representation of INDIA and it's states, and is neither drawn to scale nor conforms to international / state borders in its entirety

Table: Jobs processsed w.r.t. states

State or Union Territory	Short Name	% Job Count
Andhra Pradesh	AP	0
Arunachal Pradesh	AR	0
Assam	AS	0.110351975
Bihar	BR	0.000959582
Chandigarh	CH	0.331055924
Chattisgarh	CG	0
National Capital Territory of Delhi	DL	12.6799217
Goa	GA	0.572870687
Gujarat	GJ	1.819368211
Haryana	HR	0.559436533
Himachal Pradesh	HP	1.419222354
Jammu and Kashmir	J&K	0
Jharkhand	JK	0.179441907
Karnataka	KA	0.295551376
Kerala	KL	0
Madhya Pradesh	MP	2.730971481
Maharashtra	MH	50.62564772
Manipur	MN	1.50558477
Meghalaya	ML	0
Mizoram	MZ	0
Nagaland	NL	0
Odisha	OD	0.043181208
Puducherry	PY	0.262925575
Punjab	PB	20.46213488
Rajasthan	RJ	0.600698576
Sikkim	SK	0
Tamil Nadu	TN	3.06394657
Telangana	TS	0.906805358
Tripura	TR	0
Uttar Pradesh	UP	0.560396116
Uttarakhand	UK	0.170805665
West Bengal	WB	1.098721836

Jobs processed

;



Disclaimer: The map depicted above is only a pictorial representation of INDIA and it's states, and is neither drawn to scale nor conforms to international / state borders in its entirety

Table: State wise projects

State or Union Territory	Short Name	Number of Projects
Andhra Pradesh	AP	0
Arunachal Pradesh	AR	0
Assam	AS	16
Bihar	BR	3
Chandigarh	CH	4
Chattisgarh	CG	0
National Capital Territory of Delhi	DL	14
Goa	GA	1
Gujarat	GJ	13
Haryana	HR	4
Himachal Pradesh	HP	5
Jammu and Kashmir	J&K	0
Jharkhand	JK	1
Karnataka	KA	24
Kerala	KL	3
Madhya Pradesh	MP	3
Maharashtra	MH	126
Manipur	MN	1
Meghalaya	ML	0
Mizoram	MZ	1
Nagaland	NL	0
Odisha	OD	4
Puducherry	PY	2
Punjab	PB	13
Rajasthan	RJ	11
Sikkim	SK	0
Tamil Nadu	TN	8
Telangana	TS	18
Tripura	TR	0
Uttar Pradesh	UP	13
Uttarakhand	UK	3
West Bengal	WB	11

Projects

Disclaimer: The map depicted above is only a pictorial representation of INDIA and it's states, and is neither drawn to scale nor conforms to international / state borders in its entirety

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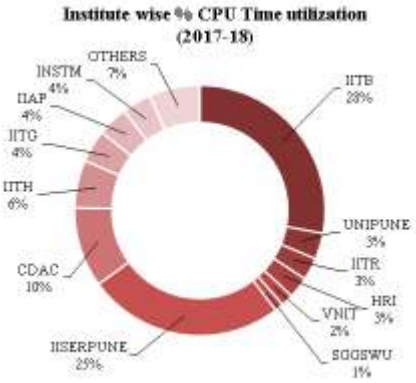
3.2 Users and Institutes

Institute wise CPU time utilization



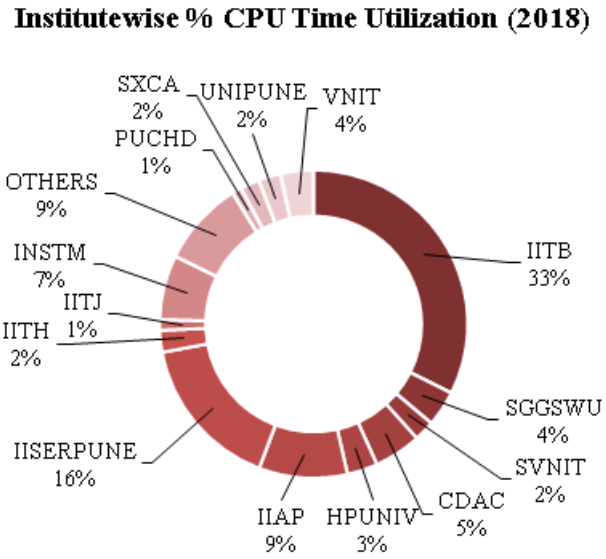


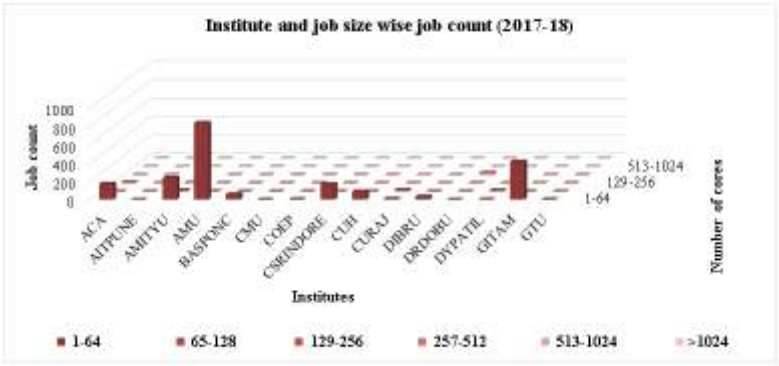
Table : Institute wise CPU time utilization Year- 2017-18

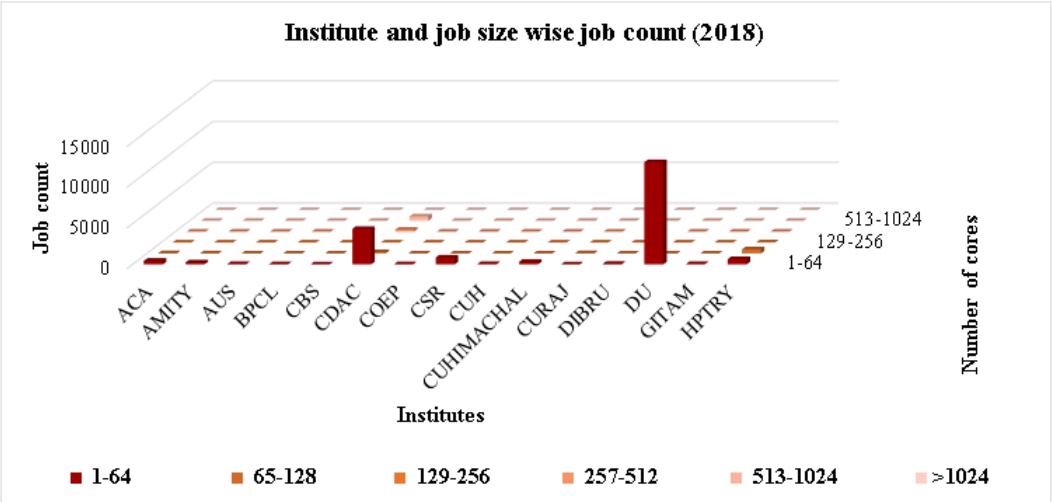
Institute Name	CPU time(seconds)
IITB	36584269805
UNIPUNE	4416978977
IITR	3772006000
HRI	3611990862
VNIT	2071074774
SGGSWU	1490835752
IISERPUNE	33166657866
CDAC	13541931387
IITH	8083505283
IITG	5492914763
IIAP	5180506080
INSTM	4956959738
OTHERS	8579338854

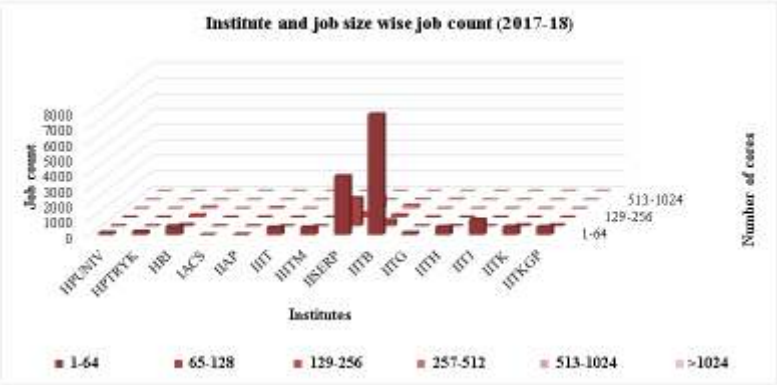
Table : Institute wise CPU time utilization Year-2018

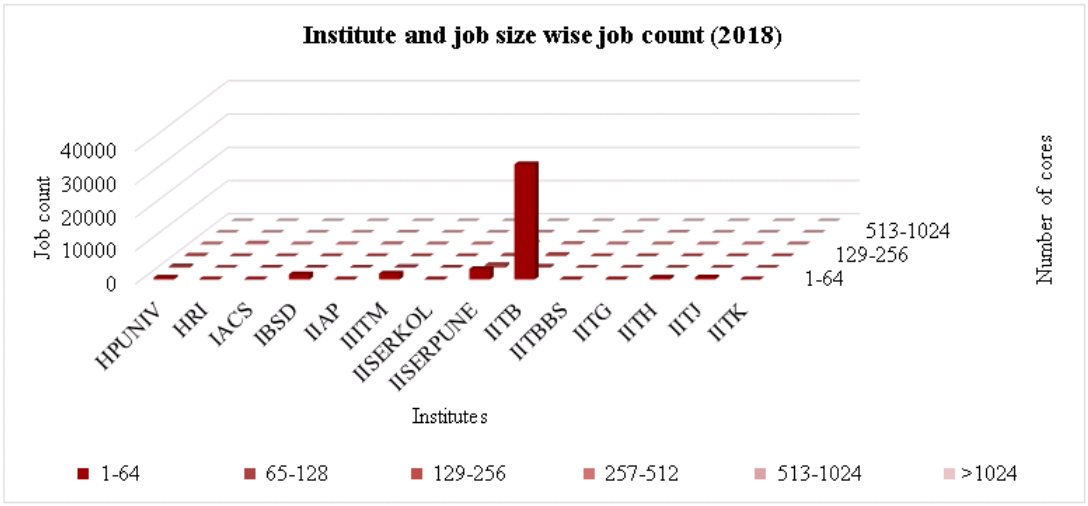
Institute	CPU time(seconds)
IITB	46090269566
SGGSWU	5344430440
SVNIT	3067733056
CDAC	7061825270
HPUNIV	4570447664
IIAP	13195440637
IISERPUNE	23221259633
IITH	3262155957
IITJ	1591580738
INSTM	9656791940
PUCHD	1439861225
SXCA	2856237025
UNIPUNE	3312310994
VNIT	4925276370
OTHERS	12704438270

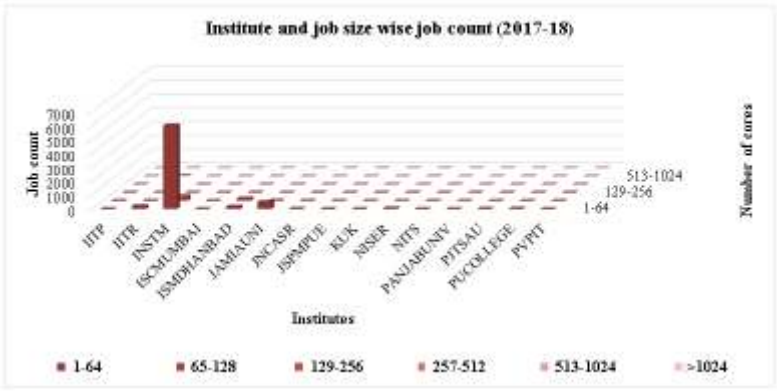
Institute and job size wise job count

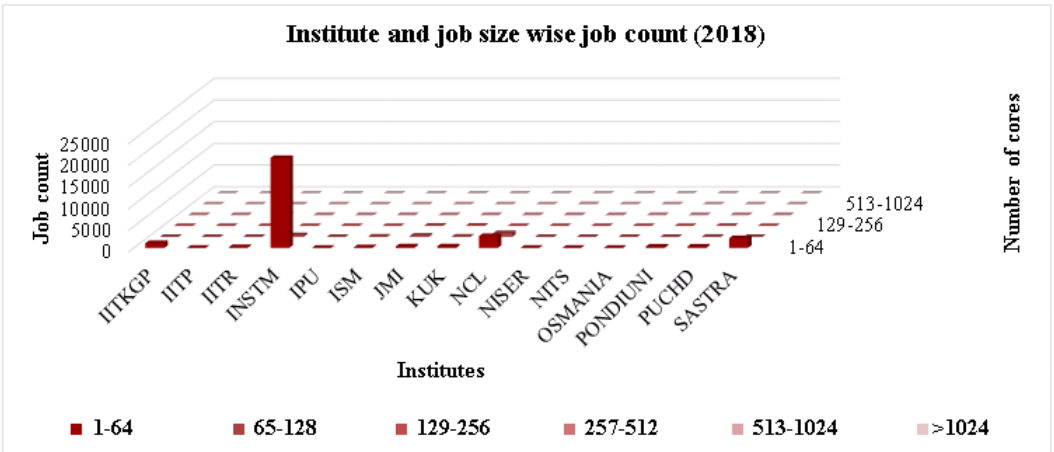


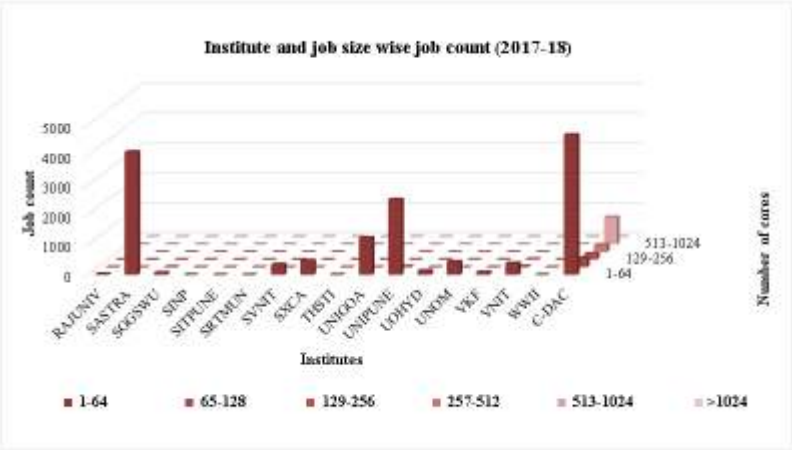



Institute and job size wise job count (2017-18)
Job count
8000
7000
6000
5000
4000
3000
2000
1000
0
HPUNIV
HPTBYK
HRI
IACS
IIAP
IIT
IIITM
IISERP
IITB
IITG
IITH
IITJ
IITK
IITKGP
513-1024
129-256
1-64
Number of cores
Institutes
1-64
65-128
129-256
257-512
513-1024
>1024


Institute and job size wise job count (2018)
Job count
40000
30000
20000
10000
0
HPUNIV
HRI
IACS
IBSD
IIAP
IIITM
IISERKOL
IISERPUNE
IITB
IITBBS
IITG
IITH
IITJ
IITK
513-1024
129-256
1-64
Number of cores
Institutes
1-64
65-128
129-256
257-512
513-1024
>1024


Institute and job size wise job count (2017-18)
Job count
7000
6000
5000
4000
3000
2000
1000
0
IITP
IITR
INSTM
ISCMUMBAI
ISMDHANBAD
JAMIAUNI
JNCASR
JSPMPUE
KUK
NISER
NITS
PANJABUNIV
PJTSAU
PUCOLLEGE
PYPT
513-1024
129-256
1-64
Number of cores
Institutes
1-64
65-128
129-256
257-512
513-1024
>1024


Institute and job size wise job count (2018)
Job count
25000
20000
15000
10000
5000
0
IITKGP
IITP
IITR
INSTM
IPU
ISM
JMI
KUK
NCL
NISER
NITS
OSMANIA
PONDIUNI
PUCHD
SASTRA
513-1024
129-256
1-64
Number of cores
Institutes
1-64
65-128
129-256
257-512
513-1024
>1024



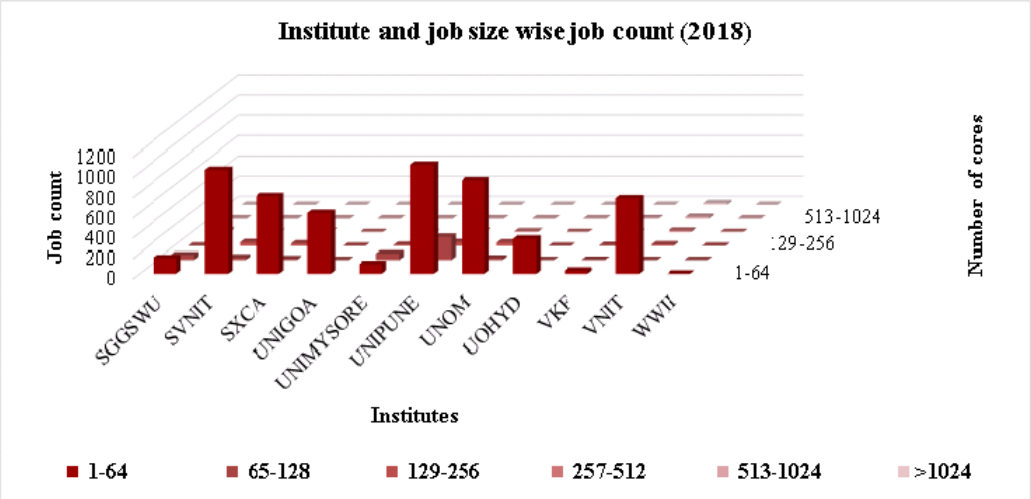


Table: Institute and Job size wise Job count Year - 2017-18

Institute	1-64	65-128	129-256	257-512	513-1024	>1024
ACA	171	0	9	0	0	0
AITPUNE	0	0	0	0	0	0
AMITYU	235	13	3	0	0	0
AMU	833	2	0	0	0	0
BASPONC	57	1	0	0	0	0
CMU	1	0	0	0	0	0
COEP	4	0	0	0	0	0
CSRINDORE	167	0	0	0	0	0
CUH	89	0	0	0	0	0
CURAJ	8	17	0	0	0	0
DIBRU	33	1	0	0	0	0
DRDOBU	0	0	1	25	0	0
DYPATIL	2	11	0	0	0	0
GITAM	413	0	0	0	0	0
GTU	3	0	0	0	0	0
HPUNIV	146	0	0	0	0	0

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Institute	**1-64**	**65-128**	**129-256**	**257-512**	**513-1024**	**>1024**
HPTRYK	217	0	0	0	0	0
HRI	569	88	152	106	0	0
IACS	1	0	0	0	0	0
IIAP	32	1	7	67	0	0
IIIT	493	1	0	0	0	0
IIITM	492	1	0	0	0	0
IISERP	3823	1825	275	747	6	0
IITB	7836	378	146	216	34	0
IITG	136	0	17	8	50	0
IITH	522	11	0	0	0	0
IITJ	997	3	0	0	0	0
IITK	531	61	0	1	0	0
IITKGP	524	61	0	0	0	0
IITP	2	0	0	0	0	0
IITR	201	5	5	6	62	0
INSTM	6015	333	5	0	0	0
ISCMUMBAI	1	0	0	0	0	0
ISMDHANBAD	161	167	16	1	0	0
JAMIAUNI	498	18	1	1	0	0
JNCASR	18	7	0	0	0	0
JSPMPUE	1	0	0	0	0	0
KUK	1	0	0	0	0	0
NISER	43	0	0	0	11	0
NITS	1	0	0	0	0	0
PANJABUNIV	1	0	0	0	0	0
PJTSAU	15	0	0	4	9	0
PUCOLLEGE	25	0	0	0	0	0
PVPIT	3	0	0	0	0	0
RAJUNIV	33	0	0	0	0	0
SASTRA	4131	0	0	0	0	0
SGGSWU	71	13	1	0	0	0
SINP	2	0	1	0	0	0
SITPUNE	1	0	0	0	0	0
SRTMUN	2	0	0	0	0	0
SVNIT	351	2	0	0	0	0
SXCA	482	1	0	1	0	0
THSTI	7	2	2	0	0	0
UNIGOA	1246	2	0	0	0	0
UNIPUNE	2534	24	1	12	0	0
UOHYD	139	0	0	0	0	0
UNOM	447	1	2	0	0	0
VKF	87	1	1	0	0	0
VNIT	394	28	18	0	3	0
WWII	2	0	0	0	0	0
C-DAC	4705	308	200	244	914	0

Table: Institute and Job size wise Job count Year - 2018

Institute	1-64	65-128	129-256	257-512	513-1024	>1024
ACA	448	31	3	0	0	0
AMITY	241	2	0	0	0	0
AUS	43	0	0	0	0	0
BPCL	14	0	0	0	0	0
CBS	1	0	0	0	0	0
CDAC	4355	159	17	233	529	0
COEP	13	0	0	0	0	0
CSR	846	0	0	0	0	0
CUH	43	0	0	0	0	0
CUHIMACHAL	323	0	0	0	0	0
CURAJ	0	28	0	0	0	0
DIBRU	60	0	0	0	0	0
DU	12544	0	0	0	0	0
GITAM	41	0	0	0	0	0
HPTRY	649	511	32	2	0	0
HPUNIV	547	431	170	8	0	0
HRI	7	1	0	300	0	0
IACS	1	7	0	0	0	0
IBSD	1535	29	2	3	0	0
IIAP	16	27	4	56	38	0
IIITM	1771	229	0	0	0	0
IISERKOL	25	15	0	0	0	0
IISERPUNE	3127	838	134	383	2	0
IITB	34637	362	348	132	53	0
IITBBS	10	0	0	0	0	0
IITG	0	0	0	0	11	0
IITH	551	6	0	0	0	0
IITJ	598	0	0	0	0	0
IITK	12	0	1	6	0	0
IITKGP	1083	14	0	0	0	0
IITP	1	0	0	0	0	0
IITR	170	0	0	0	8	0
INSTM	20707	386	12	0	0	0
IPU	3	0	0	0	0	0
ISM	112	75	0	0	0	0
JMI	329	281	57	0	0	0
KUK	317	78	89	8	4	0
NCL	2717	888	2	0	0	0
NISER	8	1	0	6	19	1
NITS	1	0	0	0	0	0
OSMANIA	6	0	0	0	0	0
PONDIUNI	274	0	0	0	0	0
PUCHD	278	20	45	2	0	0
SASTRA	2215	0	0	0	0	0
SGGSWU	153	48	1	17	0	0
SVNIT	1025	25	36	2	0	0
SXCA	764	10	24	10	0	0

Continued on next page

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Institute	1-64	65-128	129-256	257-512	513-1024	>1024
UNIGOA	597	0	0	0	0	0
UNIMYSORE	95	62	10	0	0	0
UNIPUNE	1076	225	37	9	1	0
UNOM	922	16	33	7	0	0
UOHYD	341	0	0	0	0	0
VKF	33	2	6	0	3	0
VNIT	743	0	14	13	16	16
WWII	2	0	0	0	0	0

Number of publications across institutes

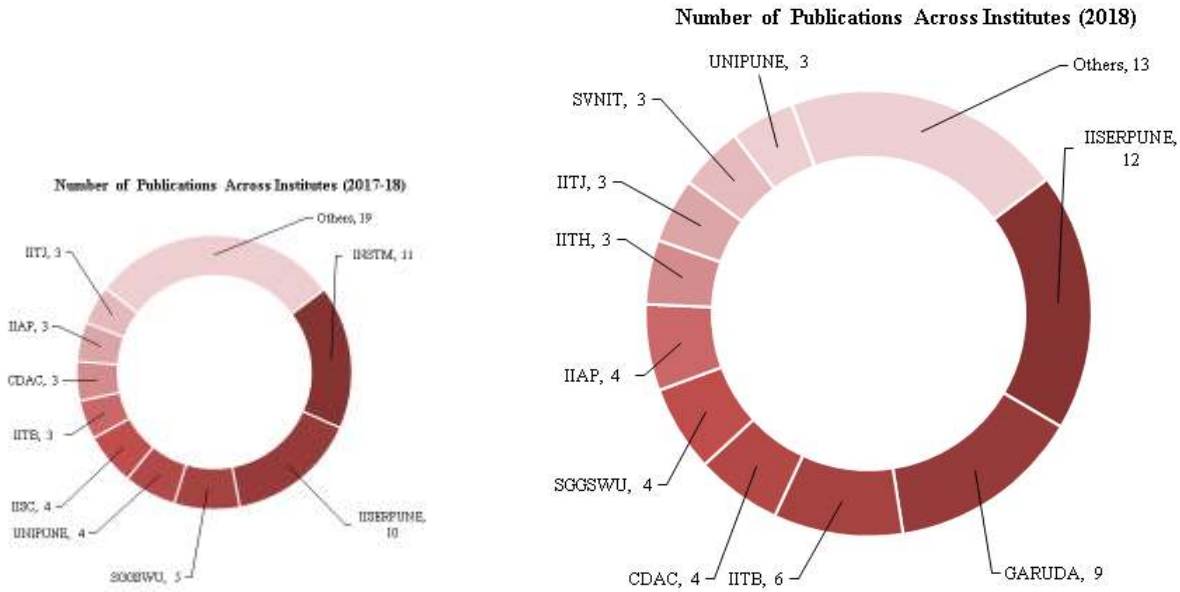


Table: Number of publications across institutes Year - 2017-18

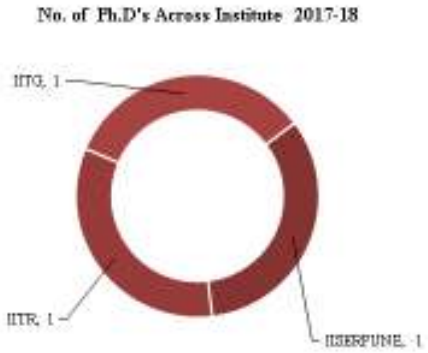
Institute	Number of Publications
INSTM	11
IISERPUNE	10
SGGSWU	5
UNIPUNE	4
IISC	4
IITB	3
CDAC	3
IIAP	3
IITJ	3
AMITYU	2
IITH	2
SVNIT	2
NCL	2
JNCASR	2
ACA	1

DYPATIL	1
BASPONC	1
UNOM	1
IISERTVM	1
IITR	1
IITG	1
NISER	1
PJTSAU	1
Total	**65**

Table: Number of publications across institutes Year-2018

Institute	**Number of Publications**
IISERPUNE	12
GARUDA	9
IITB	6
CDAC	4
IIAP	4
SGGSWU	4
IITH	3
IITJ	3
SVNIT	3
UNIPUNE	3
BASPONC	2
INSTM	2
IIITM	1
IISC	1
IISERTVM	1
IIT KGP	1
IITR	1
IITG	1
NISER	1
PONDIUNI	1
SASTRA	1
Total	**64**

Number of Ph.D's across institutes



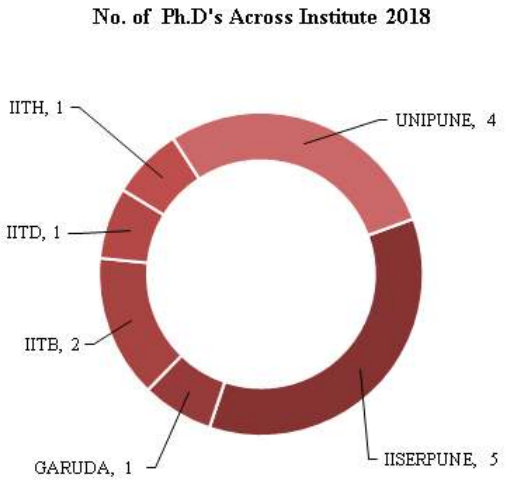


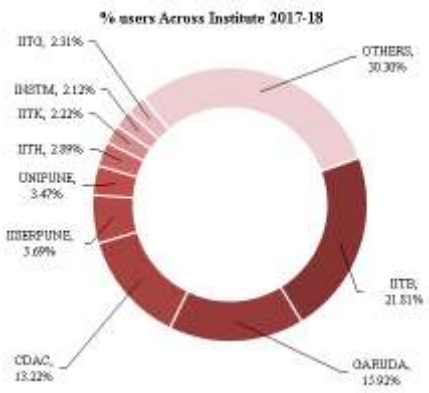
Table: Number of Ph.D's across institutes Year - 2017-18

Institute	**Number of Ph.D's**
IISERPUNE	1
IITR	1
IITG	1
Total	**3**

Table: Number of Ph.D's across institutes Year - 2018

Institute	**Number of Ph.D's**
IISER PUNE	5
GARUDA	1
IITB	2
IITD	1
IITH	1
UNIPUNE	4
IITG	1
Total	**15**

Number of Ph.D's across institutes



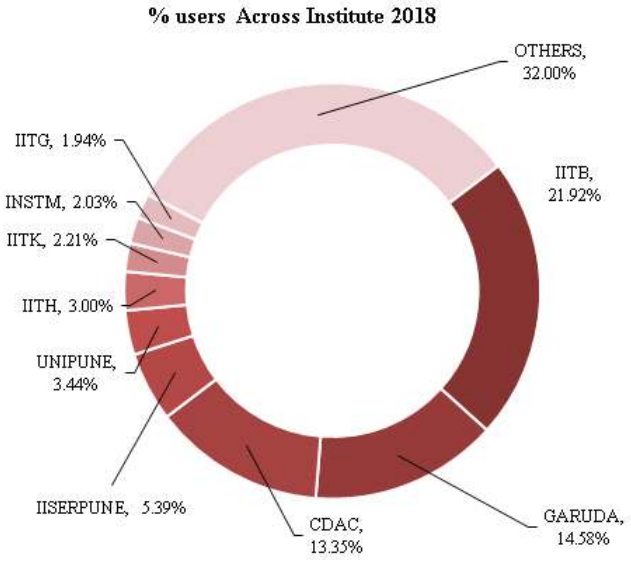


Table: Number of users across institutes Year - 2017-18

Institute	**Number of Users**
IITB	226
GARUDA	165
CDAC	137
IISERPUNE	59
UNIPUNE	36
IITH	30
IITK	23
INSTM	22
IITG	24
OTHERS	314
Total	**1036**

Table: Number of users across institutes Year - 2018

Institute	**Number of Users**
IITB	248
GARUDA	165
CDAC	151
IISERPUNE	61
UNIPUNE	39
IITH	34
IITK	25
INSTM	23
IITG	22
OTHERS	362
Total	**1130**

Table: State wise NPSF Users and Institutes

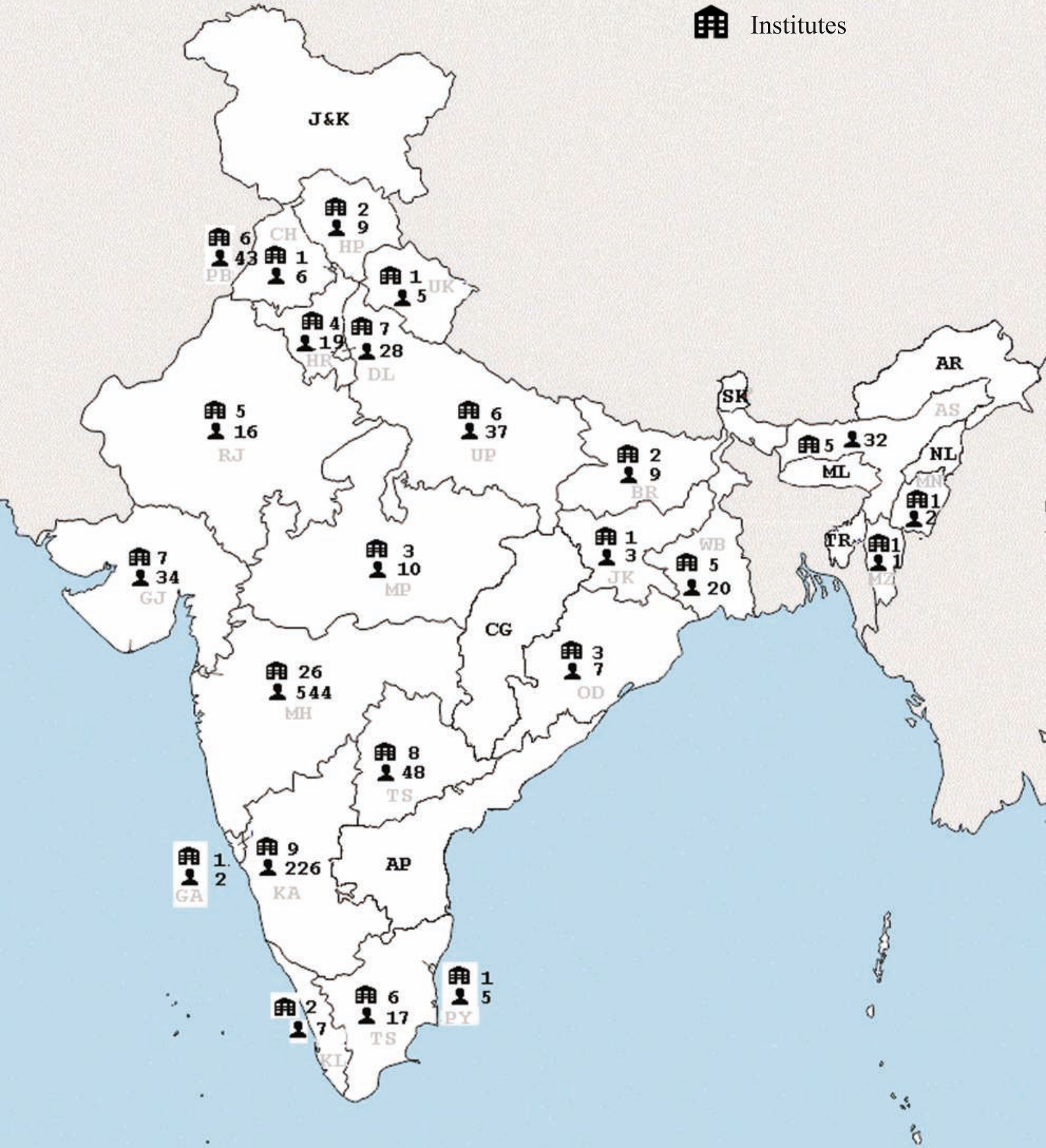
State or Union Territory	**Short Name**	**No. of Institutions**	**No. of Users**
Andhra Pradesh	AP	0	0
Arunachal Pradesh	AR	0	0
Assam	AS	5	32
Bihar	BR	2	9
Chandigarh	CH	1	6
Chattisgarh	CG	0	0
National Capital Territory of Delhi	DL	7	28
Goa	GA	1	2
Gujarat	GJ	7	34
Haryana	HR	4	19
Himachal Pradesh	HP	2	9
Jammu and Kashmir	J&K	0	0
Jharkhand	JK	1	3
Karnataka	KA	9	226
Kerala	KL	2	7
Madhya Pradesh	MP	3	10
Maharashtra	MH	26	544
Manipur	MN	1	2
Meghalaya	ML	0	0
Mizoram	MZ	1	1
Nagaland	NL	0	0
Odisha	OD	3	7
Puducherry	PY	1	5
Punjab	PB	6	43
Rajasthan	RJ	5	16
Sikkim	SK	0	0
Tamil Nadu	TN	6	17
Telangana	TS	8	48
Tripura	TR	0	0
Uttar Pradesh	UP	6	37
Uttarakhand	UK	1	5
West Bengal	WB	5	20

Users & Institutes

;

Users

Institutes



Disclaimer: The map depicted above is only a pictorial representation of INDIA and it's states, and is neither drawn to scale nor conforms to international / state borders in its entirety

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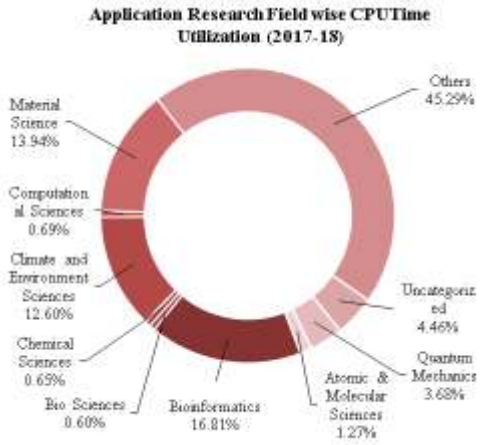
3.3 Research Field

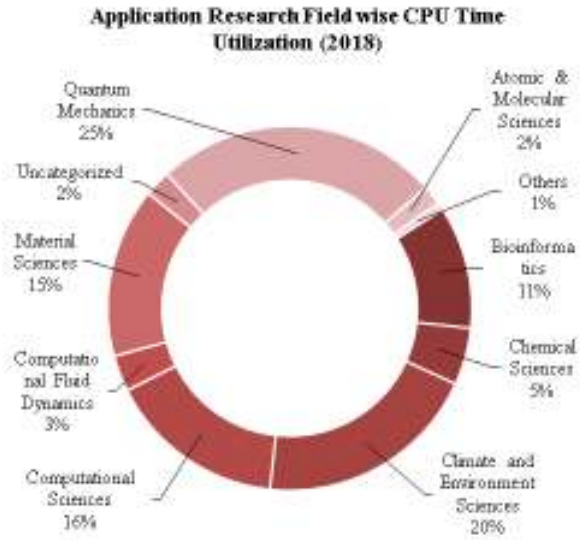
User's when affiliated with NPSF are classified according to their 1) Research Field, and 2) Institute. Former is deduced from area of work/application, whereas Institute is one of the attribute in Technical Affiliation Scheme (TAS) form. In this section, we have presented CPU time distribution, job count, and job size distribution across various Research Fields and Institutes. The inferences that can be derived from this data are to assess and corroborate percolation of HPC across application Research Fields and whether or not usage is perpetual during previous and current year. Job size distribution can be used to determine leaning towards capacity or capability computing requirements from HPC systems.

Table : List of application research fields on NPSF

S.No.	Research Field
1	Astronomy & Astrophysics
2	Atomic & Molecular Sciences
3	Bio Sciences
4	Bioinformatics
5	Chemical Sciences
6	Climate & Environment Sciences
7	Complex Systems and Statistical Physics
8	Computational Fluid Dynamics
9	Computational Physics
10	Computational Sciences
11	Data analytics
12	Geological Sciences
13	Material Sciences
14	Structural Engineering Mechanics
15	Uncategorized

Research Field wise CPU time utilization



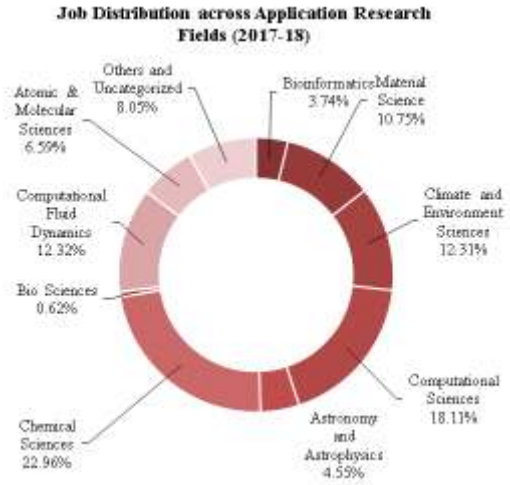


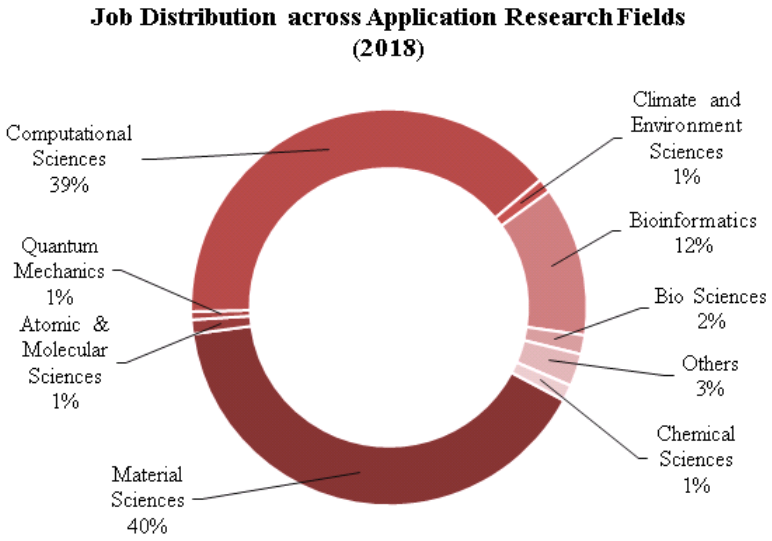
Above plots brings forth CPU time distribution across various application research fields.

Table: Research Field wise CPU time utilization

	CPU time in seconds	
Application Research Field	**2017-18**	**2018**
Astronomy and Astrophysics	0	0
Atomic & Molecular Science	552104334	344281833
Bio Science	259768576	124189101
Bioinformatics	7297809945	2117376137
Chemical Science	284302966	980810092
Climate and Environment Science	5473111638	3864861304
Complex Systems and Statistical Physics	0	0
Computational Fluid Dynamics	154974099	621817044
Computational Physics	0	0
Computational Science	301228639	3066884362
Data analytics	1144878	154016
Geological Science	3037660	179280
Material Science	6051030366	2930470531
Quantum Mechanics	1596156672	4886325127
Structural / Engineering Mechanics	19760	0
Uncategorized	1938219316	450640283

Job distribution across application research fields



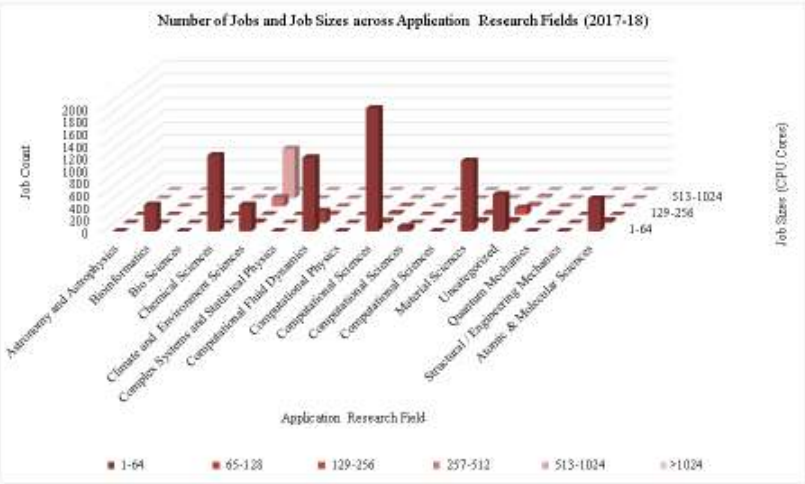


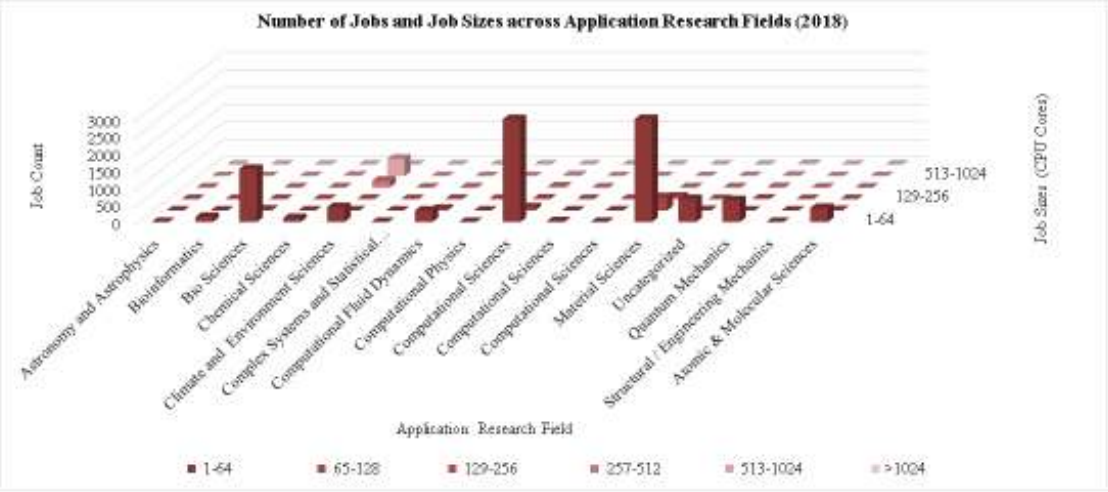
Above plots shows application research fields wise percentage distribution of number of jobs processed.

Table:Job distribution across application research fields

	No. of Jobs	
Application Research Field	**2017-18**	**2018**
Astronomy and Astrophysics	0	182
Atomic & Molecular Science	573	1199
Bio Science	26	1620
Bioinformatics	428	12751
Chemical Science	1245	1359
Climate and Environment Science	1408	1191
Complex Systems and Statistical Physics	0	99
Computational Fluid Dynamics	1407	398
Computational Physics	0	5
Computational Science	2071	40871
Data analytics	77	19
Geological Science	13	6
Material Science	1229	41761
Quantum Mechanics	21	690
Structural / Engineering Mechanics	1	0
Others & Uncategorized	808	2061

Job sizes across application research fields





Above plots depicts distribution of jobs in reference to number of CPU cores requested, binned by ranges 1-64, 65-128, 129-256, 257-512, and 513-1024 & above.

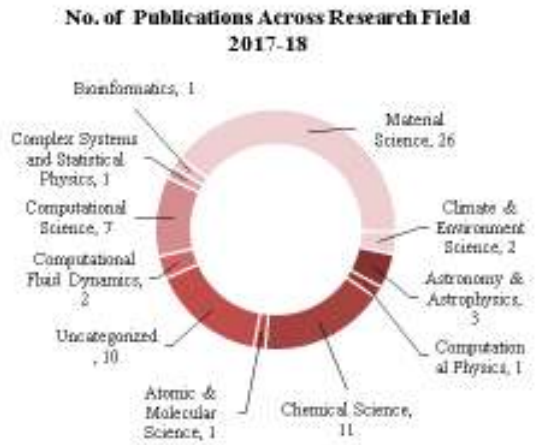
Table: Number of Jobs and Job Sizes across Application Research Fields (2017-18)

Application Research Fields	**1-64**	**65-128**	**129-256**	**257-512**	**513-1024**	**>1024**
Astronomy and Astrophysics	0	0	0	0	0	0
Atomic & Molecular Science	529	44	0	0	0	0
Bioinformatics	428	0	0	0	0	0
Bio Science	0	0	1	25	0	0
Chemical Science	1230	1	1	4	9	0
Climate and Environment Science	429	25	5	148	801	0
Complex Systems and Statistical Physics	0	0	0	0	0	0
Computational Fluid Dynamics	1196	197	13	0	1	0
Computational Physics	0	0	0	0	0	0
Computational Science	1990	35	26	15	5	0
Computational Science	77	0	0	0	0	0
Computational Science	2	11	0	0	0	0
Material Science	1140	42	34	8	5	0
Quantum Mechanics	0	0	18	0	3	0
Structural / Engineering Mechanics	1	0	0	0	0	0
Uncategorized	599	45	112	25	27	0

Table: Number of Jobs and Job Sizes across Application Research Fields 2018

Application Research Fields	**1-64**	**65-128**	**129-256**	**257-512**	**513-1024**	**>1024**
Astronomy and Astrophysics	0	0	0	0	0	0
Atomic & Molecular Science	407	14	0	0	0	0
Bioinformatics	152	0	0	0	0	0
Bio Science	1535	29	2	3	0	0
Chemical Science	117	0	0	6	16	0
Climate and Environment Science	431	4	1	196	499	0
Complex Systems and Statistical Physics	0	0	0	0	0	0
Computational Fluid Dynamics	335	53	4	6	0	0
Computational Physics	0	0	0	0	0	0
Computational Science	2966	96	13	30	22	0
Computational Science	19	0	0	0	0	0
Computational Science	0	6	0	0	0	0
Material Science	2972	385	68	5	3	0
Quantum Mechanics	631	0	14	13	16	16
Structural / Engineering Mechanics	0	0	0	0	0	0
Uncategorized	666	13	0	7	8	0

Number of publicatons across research fields



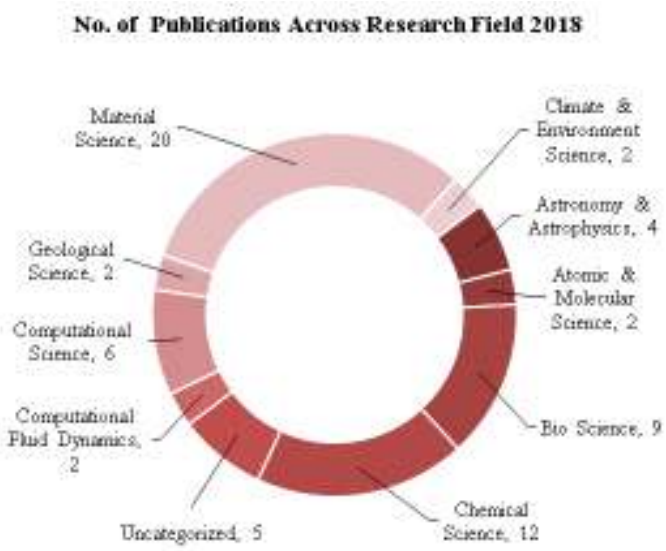
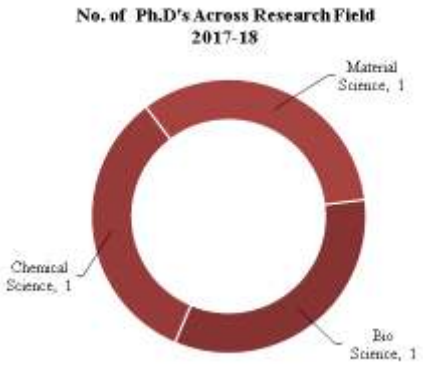


Table: Number of publicatons across research fields

	Number of publicatons	
Application Research Fields	**2017-18**	**2018**
Astronomy & Astrophysics	3	4
Atomic & Molecular Science	1	2
Bioinformatics	1	0
Bio Science	0	9
Chemical Science	11	12
Climate & Environment Science	2	2
Complex Systems and Statistical Physics	1	0
Computational Fluid Dynamics	2	2
Computational Physics	1	0
Computational Science	7	6
Geological Science	0	2
Material Science	26	20
Uncategorized	10	5
Total	**65**	**64**

Number of PhDs across research fields



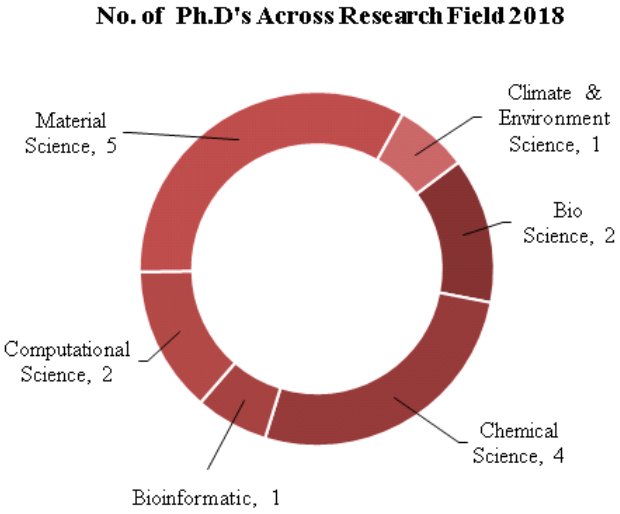
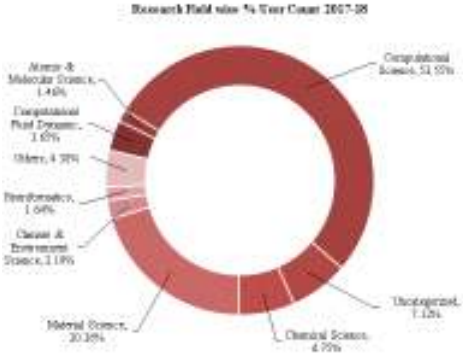


Table: Number of PhDs across research fields

	Number of PhDs	
Application Research Fields	**2017-18**	**2018**
Bio Science	1	2
Chemical Science	1	4
Bioinformatic	0	1
Computational Science	0	2
Material Science	1	5
Climate & Environment Science	0	1
Total	**3**	**15**

Number of users across research fields



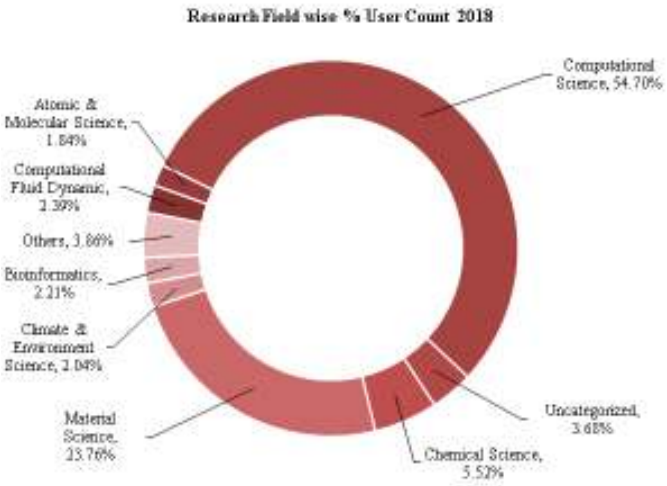


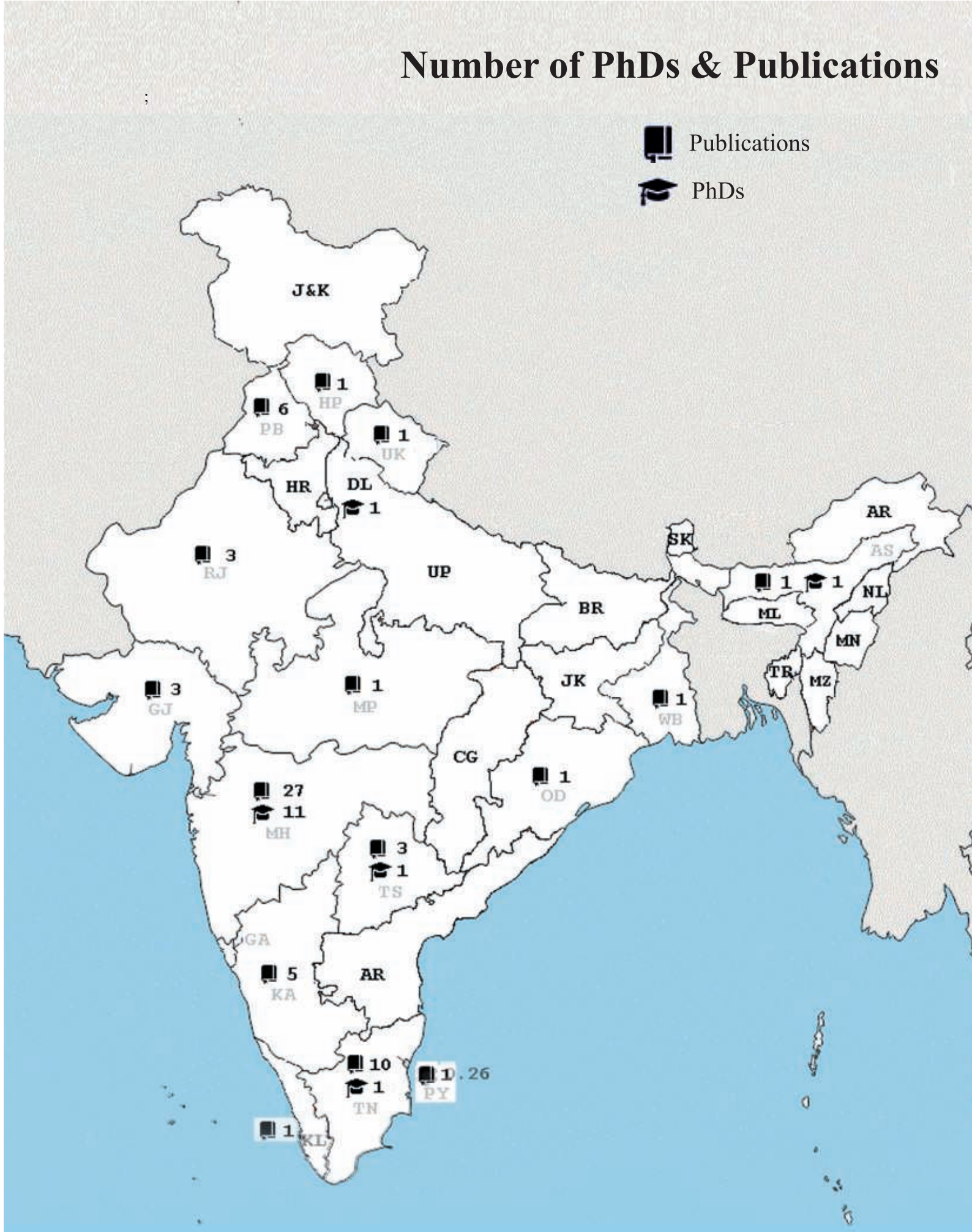
Table: Number of users across research fields

	Number of Users	
Application Research Fields	**2017-18**	**2018**
Astronomy and Astrophysic	3	3
Atomic & Molecular Science	8	10
Bio Science	6	6
Bioinformatic	9	12
Chemical Science	37	30
Climate and Environment Science	12	11
Complex Systems and Statistical Physic	1	1
Computational Fluid Dynamic	20	13
Computational Physics	1	1
Computational Science	288	297
Data analytic	1	2
Geological Science	6	6
Material Science	111	129
Quantum Mechanic	2	2
Structural / Engineering Mechanic	4	0
Uncategorized	39	20
Total	**548**	**543**

Table: State wise Number of Publications and PhDs

State or Union Territory	**Short Name**	**No. of Publi-cations**	**No. of PhDs**
Andhra Pradesh	AP	0	0
Arunachal Pradesh	AR	0	0
Assam	AS	1	1
Bihar	BR	0	0
Chandigarh	CH	0	0
Chattisgarh	CG	0	0
National Capital Territory of Delhi	DL	0	1
Goa	GA	0	0
Gujarat	GJ	3	0
Haryana	HR	0	0
Himachal Pradesh	HP	0	0
Jammu and Kashmir	J&K	0	0
Jharkhand	JK	0	0
Karnataka	KA	5	0
Kerala	KL	1	0
Madhya Pradesh	MP	1	0
Maharashtra	MH	27	11
Manipur	MN	0	0
Meghalaya	ML	0	0
Mizoram	MZ	0	0
Nagaland	NL	0	0
Odisha	OD	1	0
Puducherry	PY	1	0
Punjab	PB	6	0
Rajasthan	RJ	3	0
Sikkim	SK	0	0
Tamil Nadu	TN	10	1
Telangana	TS	3	1
Tripura	TR	0	0
Uttar Pradesh	UP	0	0
Uttarakhand	UK	1	0
West Bengal	WB	1	0

Number of PhDs & Publications



Disclaimer: The map depicted above is only a pictorial representation of INDIA and it's states, and is neither drawn to scale nor conforms to international / state borders in its entirety

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3.4 Queue

Job Submission Queues

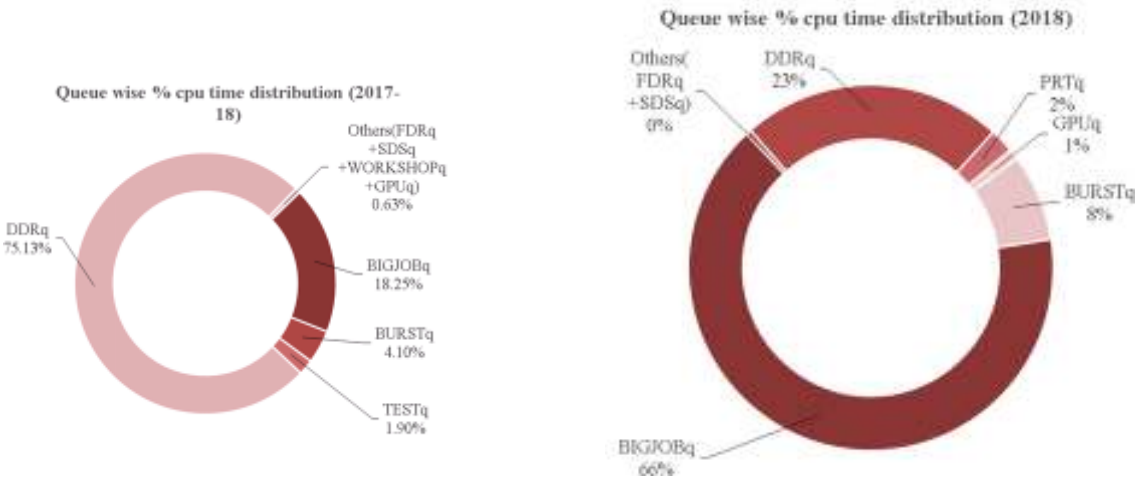
Various queues ensures a spectrum of quality of service according to the resource requirement of the users for different computing exercises. Below table shows the summary of job submission queues.

Table : Summary of queues on NPSF

Queue	**Wall Time Limit**	**Accelerator(s) in the nodes in the partition**
batch	7 Days	Xeon Phi
TESTq	2 Hours	Xeon Phi
GPUq	7 Days	GPU
SDSq	06 Hours	Xeon Phi
BURSTq	17 Hours 55 Minutes	Xeon Phi
BIGJOBq	7 Days	Xeon Phi
PRTq	7 Days	Xeon Phi

- TESTq: The users get resources without having to wait longer to run the test jobs before the actual job runs. Currently the maximum allowed walltime for TESTq queue is 2 Hrs per job.
- GPUq: Queue for jobs with GPU nodes/SMP node.
- SDSq: Queue for jobs on resources with advanced reservation. The resources in under SDSq are primarily for running the production jobs on daily basis for a fixed duration as per the commitment to different users.
- BURSTq: Queue for jobs requiring large number of cores for less wall time.
- BIGJOBq: Queue for jobs requiring large number of cores for less wall time.
- PRTq: Queue for jobs with higher priority.

Distribution of CPU time utilization w.r.t. Job queues

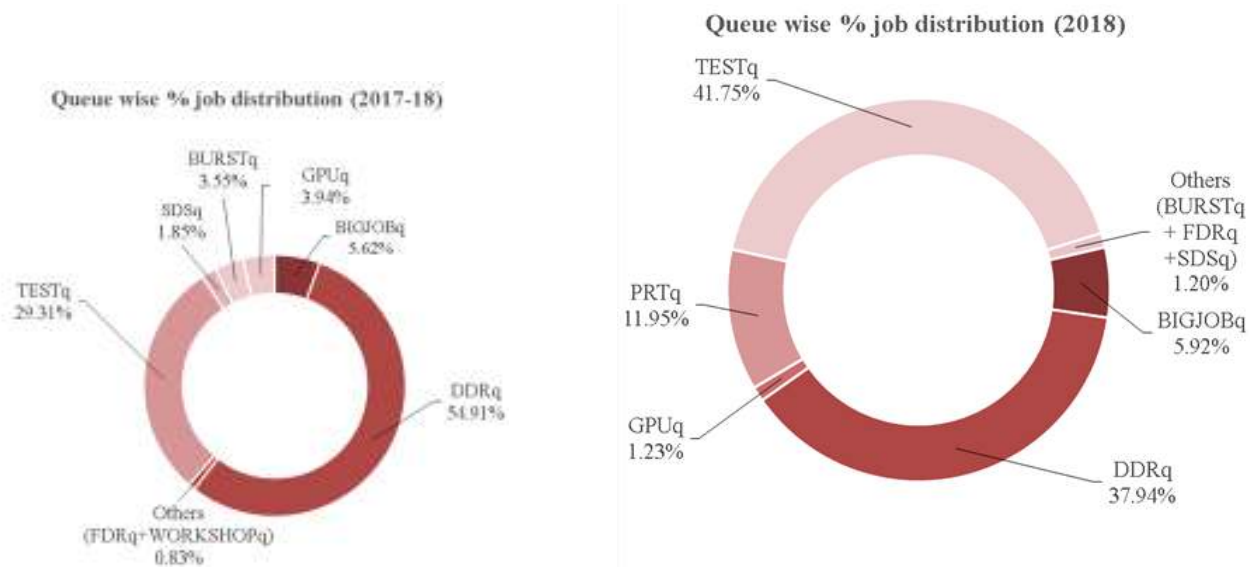


Above graph shows distribution in percentage of CPU time utilized by jobs in respective queues.

Table: Queue wise cpu time distribution

	CPU Time (Hours)	
Queue	**2017-18**	**2018**
BIGJOBq	39607197720	25595859.52
BURSTq	8902900224	3008838.749
DDRq	163082517696	9035466.181
FDRq	15204	960.808
GPUq	588302112	364162.744
PRTq	0	841979.58
SDSq	769674332	170208.331
TESTq	4124914568	499686.026
WORKSHOPq	946974	0

Distribution of jobs w.r.t. queues

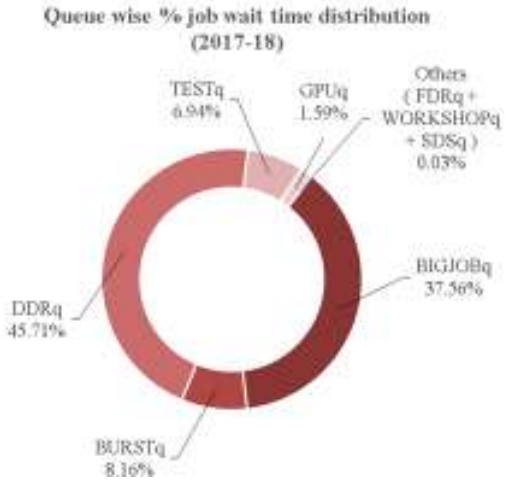


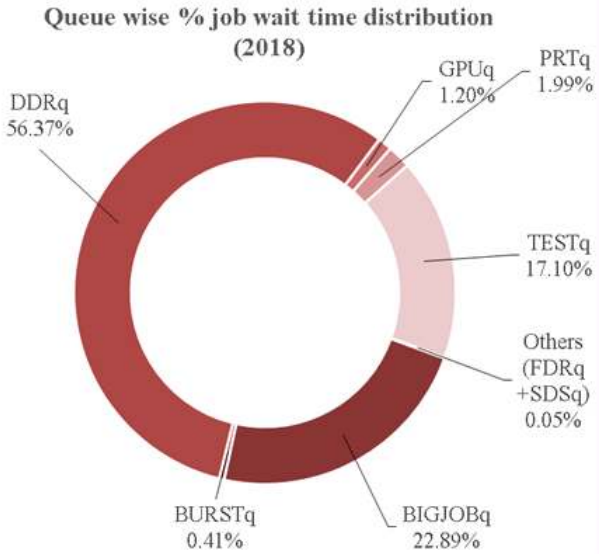
Above graph shows distribution in percentage of jobs among execution queues.

Table: Queue wise jobs distribution

	Number of jobs	
Queue	**2017-18**	**2018**
BIGJOBq	2390	6168
BURSTq	1513	921
DDRq	23370	39541
FDRq	61	204
GPUq	1675	1287
PRTq	0	12449
SDSq	787	129
TESTq	12477	43512
WORKSHOPq	291	0

Distribution of wait time w.r.t. queues



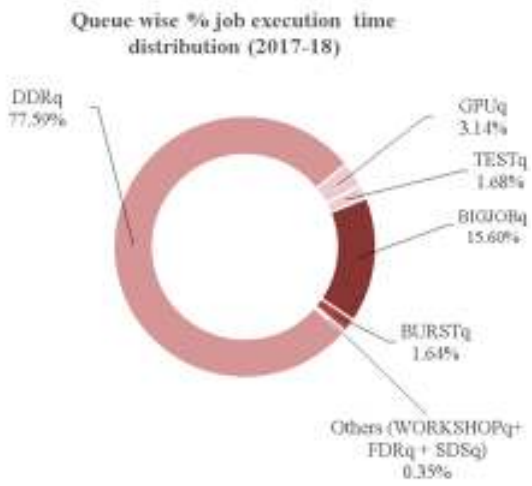


Above graph is a representation of percentage distribution of time spent by jobs, once submitted, until allowed for execution on system. Due to restriction of maximum walltime for a job as per policy, jobs submitted to TESTq experience least wait.

Table: Queue wise Wait Time distribution

	Wait Time (Hours)	
Queue	**2017-18**	**2018**
BIGJOBq	450482.0942	430203.969
BURSTq	97860.94333	7709.271
DDRq	548202.7439	1059568.325
FDRq	11.82888889	857.976
GPUq	19122.91639	22520.742
PRTq	0	37444.241
SDSq	352.0522222	69.779
TESTq	83236.03667	321400.491
WORKSHOPq	4.616666667	0

Distribution of execution time w.r.t. queues



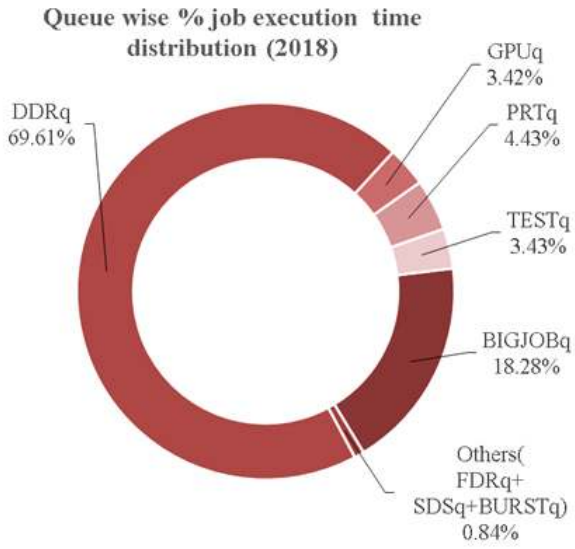


Table: Queue wise job execution time distribution

	Execution Time (Hours)	
Queue	**2017-18**	**2018**
BIGJOBq	83623.64222	118777.135
BURSTq	8784.050556	5020.644
DDRq	415908.1244	452364.064
FDRq	28.485	77.911
GPUq	16851.57833	22231.962
PRTq	0	28781.022
SDSq	1708.120278	359.151
TESTq	9014.130556	22262.192
WORKSHOPq	147.8691667	0

Queue vs Jobs wait time / execution time ratio

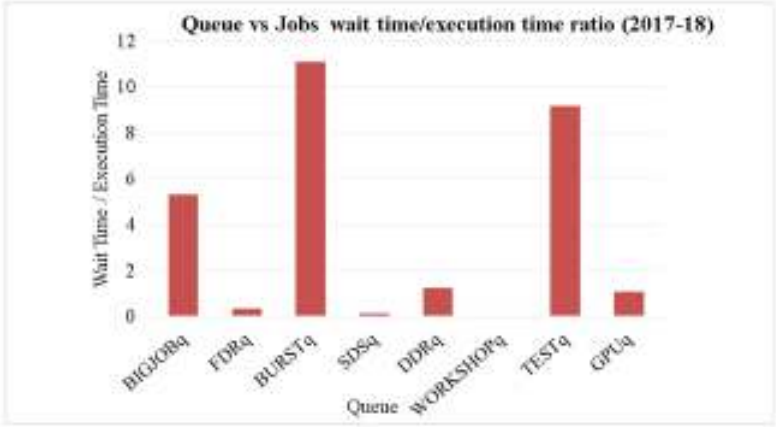
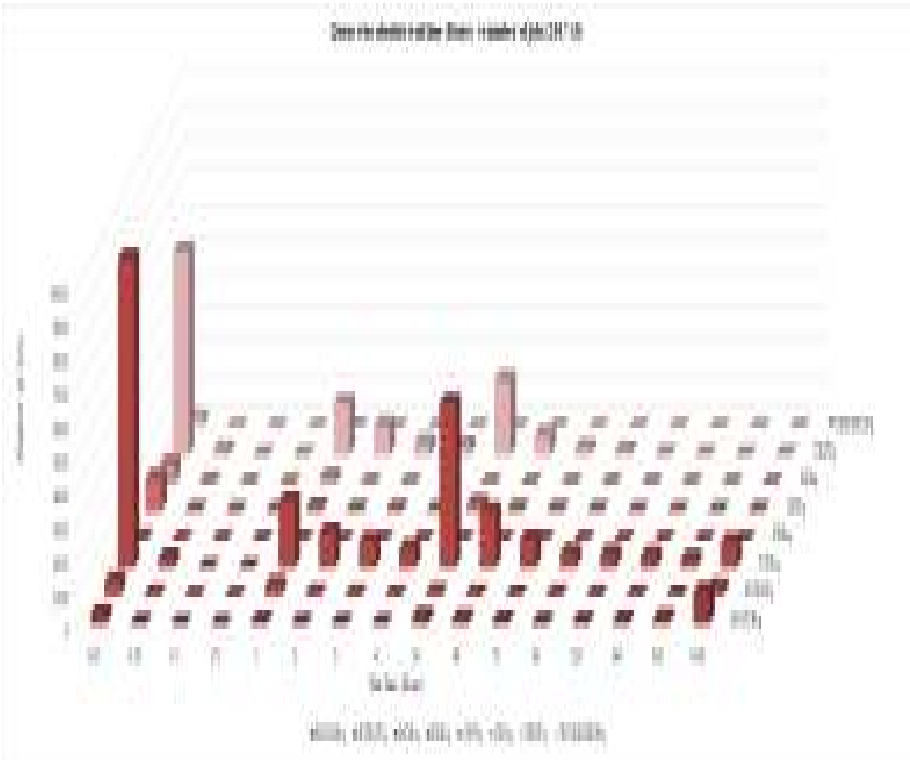


Table: Queue wise Wait Time/Execution distribution

	Wait Time / Execution Time ratio	
Queue	**2017-18**	**2018**
BIGJOBq	5.387018338	3.621942632
BURSTq	11.14075366	1.535514368
DDRq	1.318086163	2.342291109
FDRq	0.415267295	11.01225758
GPUq	1.134784885	1.012989407
PRTq	0	1.301004565
SDSq	0.206105054	0.194288753
TESTq	9.233950646	14.43705503
WORKSHOPq	0.031221294	0

Queue wise absolute wait time(Hours) vs number of jobs



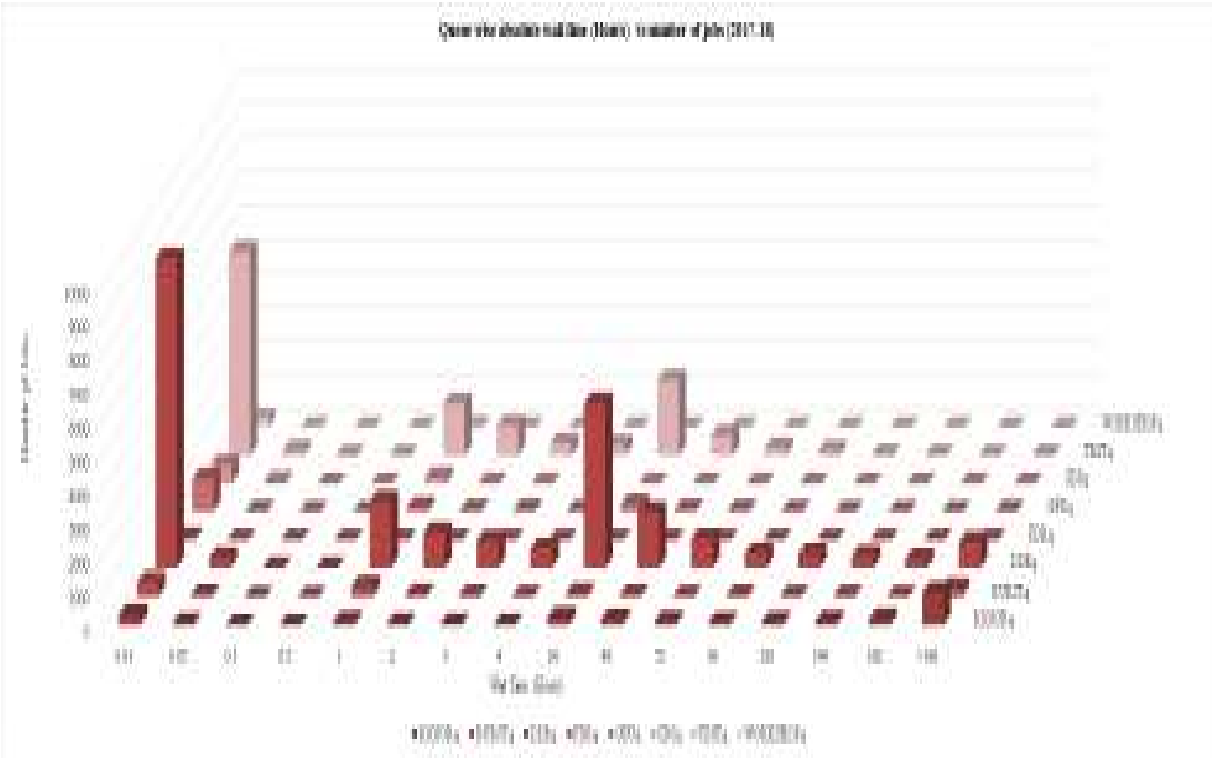


Table: Queue wise absolute wait time (Hours) vs number of jobs (2017-18)

2017-18	0.01	0.05	0.1	0.5	1	2	3	4	24	48	72	96	120	144	168	>168
BIGJOBq	313	39	0	0	90	32	28	17	223	162	100	65	83	104	173	961
BURSTq	435	57	0	0	324	70	49	26	97	50	26	46	30	34	24	245
DDRq	9128	299	0	0	1970	1031	808	565	4857	1643	853	425	410	353	258	770
FDRq	51	1	0	0	6	1	0	1	1	0	0	0	0	0	0	0
GPUq	975	30	0	0	128	51	59	33	217	63	45	30	7	6	8	23
SDSq	550	44	0	0	172	9	1	0	5	5	0	1	0	0	0	0
TESTq	6021	145	0	0	1533	883	364	309	2224	595	214	135	22	16	2	14
WORKSHOPq	255	8	0	0	28	0	0	0	0	0	0	0	0	0	0	0

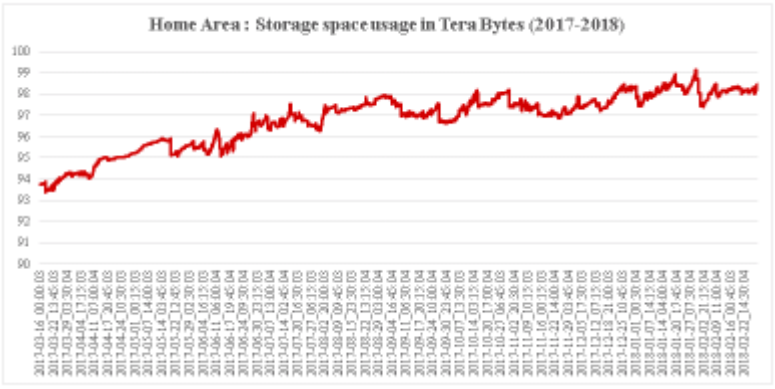
Table: Queue wise absolute wait time (Hours) vs number of jobs (2018)

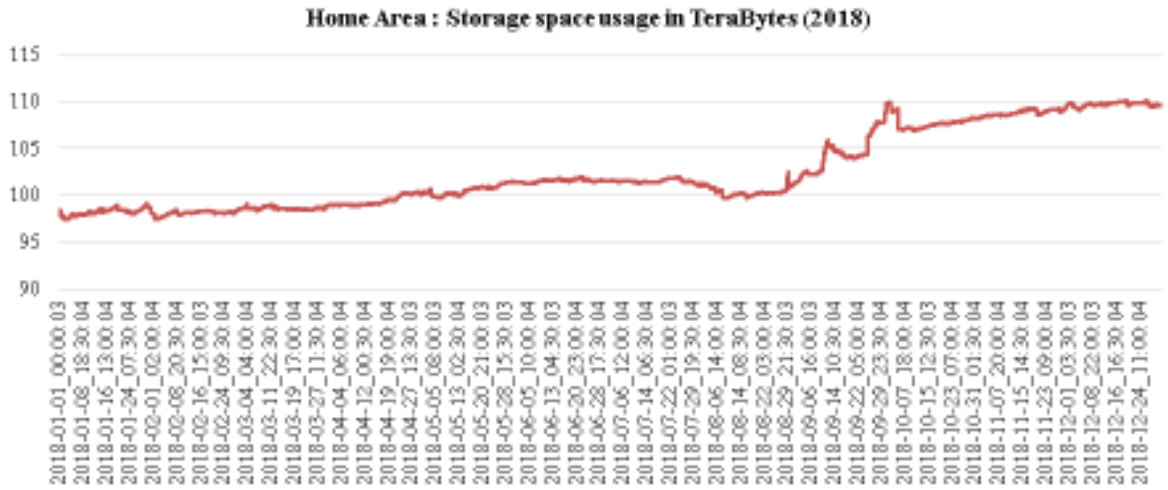
2018	0.01	0.05	0.1	0.5	1	2	3	4	24	48	72	96	120	144	168	>168
BIGJOBq	2209	105	0	0	546	232	151	112	1051	414	258	119	144	69	171	587
BURSTq	305	42	0	0	359	73	42	21	25	14	4	9	8	1	2	16
DDRq	11098	401	0	0	3606	2540	1718	1364	9631	3573	1844	822	617	633	457	1237
FDRq	174	4	0	0	15	3	1	1	4	1	0	0	0	0	0	1
GPUq	518	11	0	0	62	36	28	23	291	168	88	30	17	11	1	3
PRTq	8590	158	0	0	573	432	361	366	1529	338	59	11	15	11	1	5
SDSq	42	4	0	0	78	1	1	0	3	0	0	0	0	0	0	0
TESTq	11323	923	0	0	6541	3602	2349	1921	13798	2365	614	22	4	2	11	37

3.5 Storage

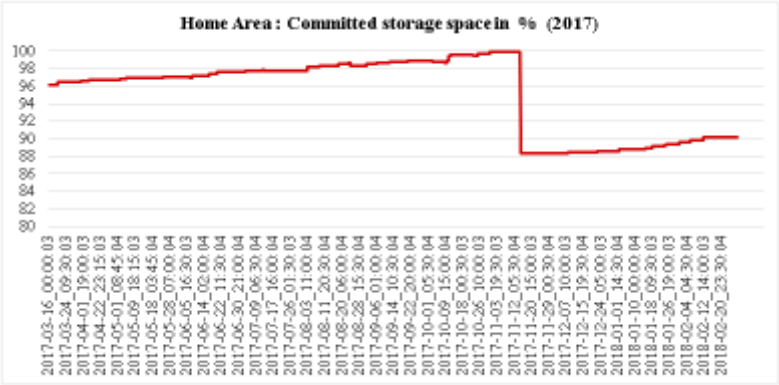
A HPC system is always coupled with one or more disk storage systems. Given the performance expected from such storage systems, they are distributed in nature, employing several I/O servers for increased throughput. At NPSF, two such storage systems are commissioned 1) Home Area, & 2) Scratch Area. Both of these said storage area are layered with POSIX compliant distributed and parallel filesystems respectively, with storage delivery over high-bandwidth, low-latency InfiniBand network. A third tape based storage system is used for scheduled backup of Home Area to mitigate data loss in event of failure.

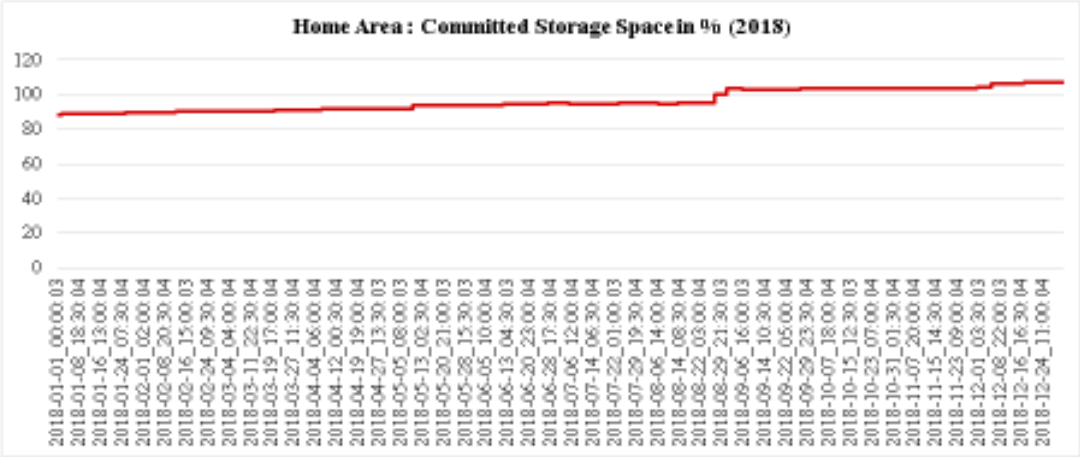
Occupancy on both 1 and 2 is governed under policies for fair usage. Scratch Area is only available during job execution and for Home Area, every user has quota allocation with default being 100GB. The statistics of the Home Area are measured in terms of 1) total occupancy in respect to size and number of files 2) committed by way of on demand quota allocation as percentage of total available, and 3) percentage change at intervals in occupancy and number of files.



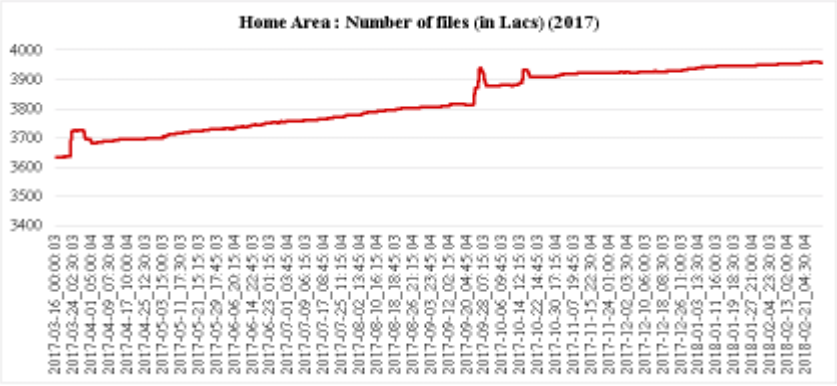


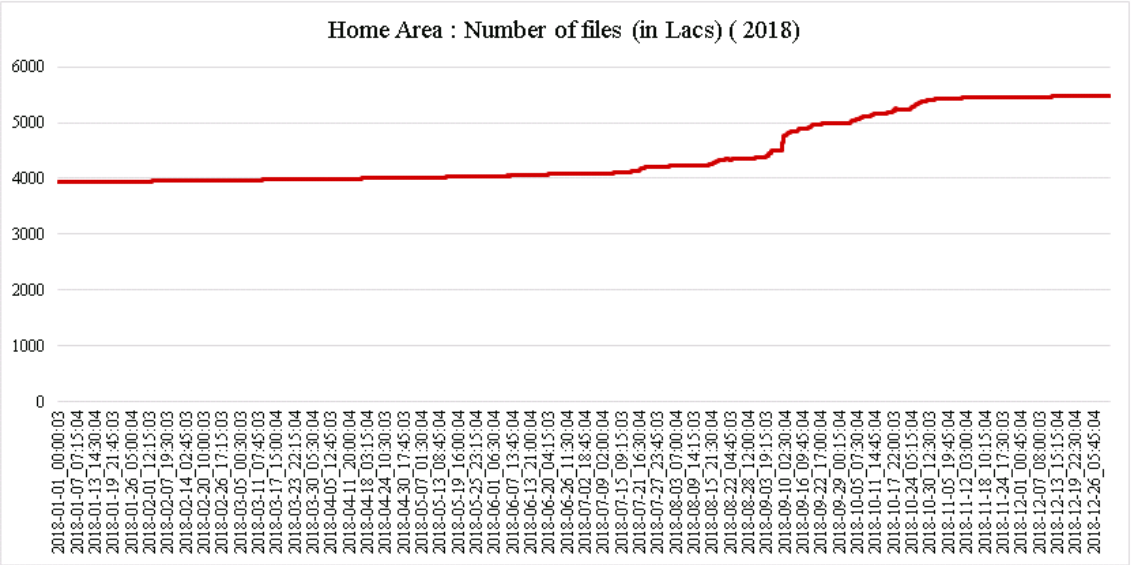
Above line plot depicts variations in total occupancy of Home Area. Total available size is 197 TB.





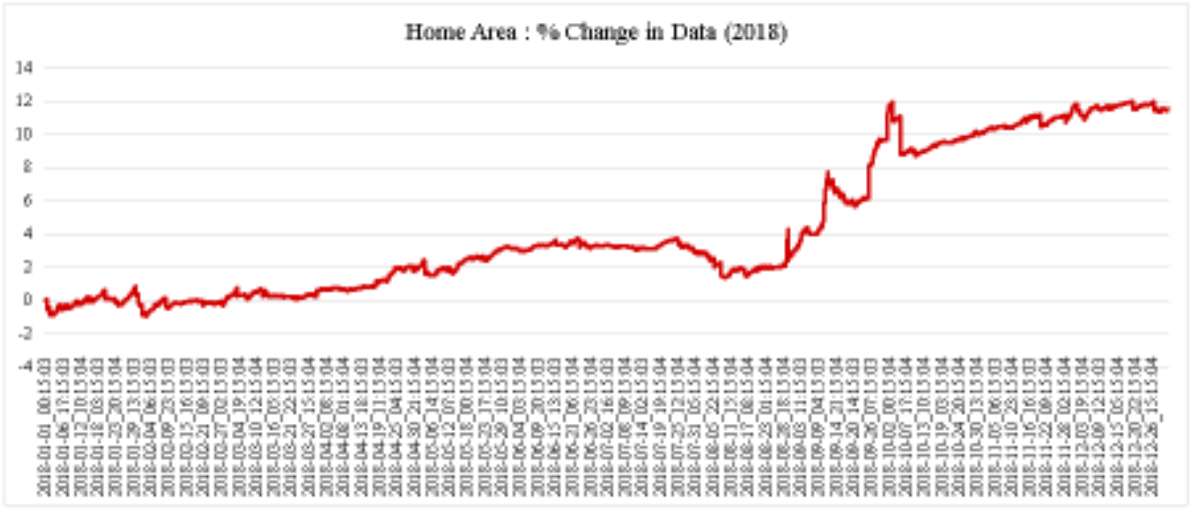
Above line plot presents total quota allocations during last year as percentage of total capacity. This can be seen as an indicator for the requirement of expansion of the storage.

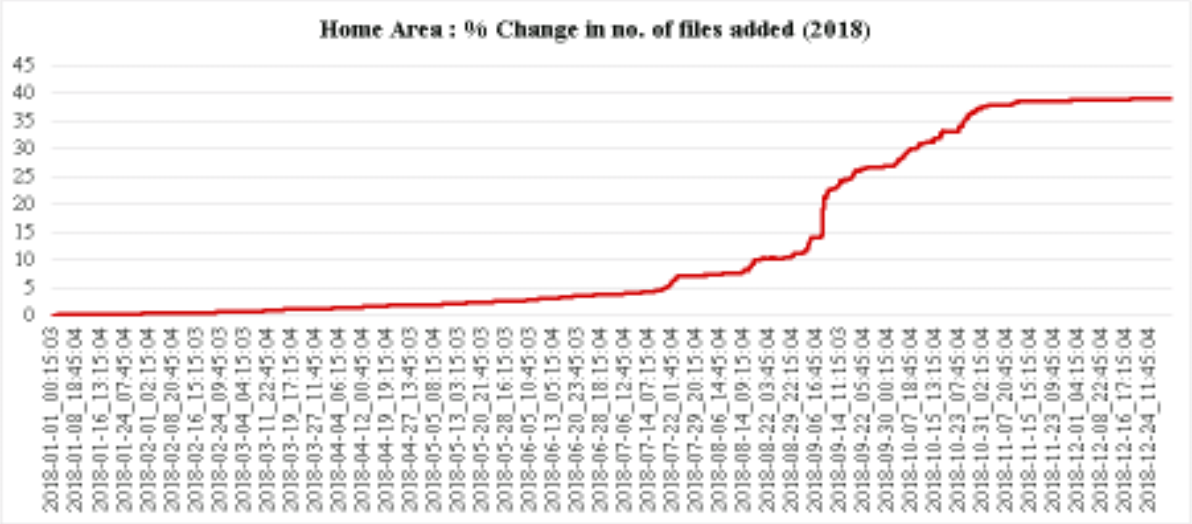




Above line plot depicts variations in occupancy of Home Area in terms of number of files.

The below statistics shows % change in data size and % change in number of files which defines the need of backing up the data at regular intervals with incremental backup. If the % change in data/ no. of files becomes equal to the actual occupied storage, then the backup policy should be changed from incremental to full dump. The above statistics shows that we can continue with the incremental backup sessions.





Overlap of three months between previous and current report is due to change in report period from Feb-Mar to Jan-Dec.

4

Science using NPSF

Some of the publication reports and work reports based on the research publication/s in high impact journals and the work that has been carried out on NPSF.

4.1 Work Reports

Title of the work carried out: Different kinds of energy conversion in 2D materials

Name & Designation of the Chief Investigator: Dr. Abir De Sarkar, Scientist-E/Assoc. Prof. & Dean (Academics)

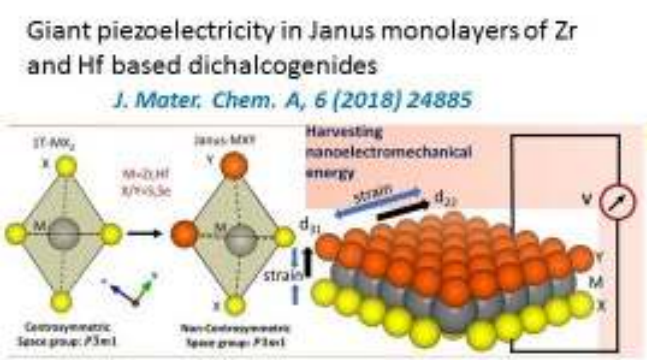
E-mail Id: abir@inst.ac.in,abirdesarkar@gmail.com

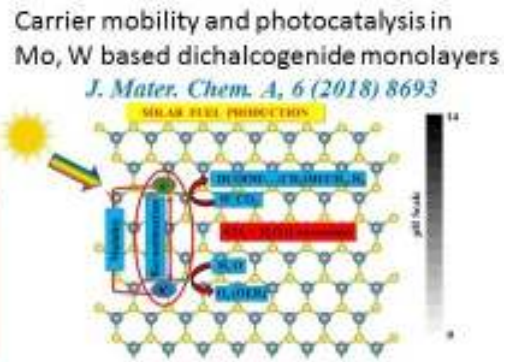
Institution Name: Institute of Nano Science and Technology (Autonomous Institute supported by the Departmentof Science and Technology,Government of India), Phase 10, Sector 64, Mohali, Punjab-160062

Research Challenge/s:

Studying large systems, which can be highly computationally intensive and demanding & also running some calculations for a long duration of time (say, more than 72 hrs)

Work carried , Milestone, Achievements & Graphs, Plots:





Publications / Articles etc. (If any):

1. Dimple, Nityasagar Jena, Ashima Rawat, Raihan Ahammed, Manish Kumar Mohanta,Abir De Sarkar*, "Emergence of high piezoelectricity along with robust electron mobility in Janus structures in semiconducting Group IVB dichalcogenide monolayers",Journal of Materials Chemistry A,6 (2018) 24885-24898 (Impact factor: 9.931)
2. Ashima Rawat, Nityasagar Jena, Dimple,Abir De Sarkar*, "A comprehensive study on carrier mobility and artificial photosynthetic properties in group VI B transition metal dichalcogenide monolayers",Journal of Materials Chemistry A,6 (2018) 8693-8704 (Impact factor: 9.931)

Awards (If any):

CNR Rao Award for Excellence in Nanoresearch for the year 2018

Work presented in conference/s with photographs (if any):

Presenting invited talk at Science Academies Lecture Workshop on Frontiers in Chemical and Material Sciences: Theory and Practice held at the North Bengal University between 8th and 10th February, 2018

Appreciation / Recognition (if any):

Have been invited to present my work at both National and International Conferences

References:

Benefits & experience of using NPSF:

PARAM Yuva II has helped me immensely in guiding my Ph.D. students and my Postdoc on a wide range of research problems. The helpdesk has responded with great promptitude in installing different programs & modules required by us from time to time. In short, helpdesk has been remarkably supportive. We owe the deepest debt of gratitude to CDAC-Pune and the support team of PARAM Yuva II.

Any other relevant information (if any):

CDAC, Pune has been doing a wonderful job for many years in helping Computational Scientists across India in their active pursuit of research. The strong computational support provided by CDAC-Pune enables us to pursue good quality research. I would like to appeal to the Govt. of India to allocate substantial funds to CDAC-Pune to support the latter in their future endeavors, which includes upgrading their HPC systems. Any HPC system gets outdated in five years. Moreover, the usage of Param Yuva II is really high. Param Yuva II caters to users from all over India. CDAC-Pune is in dire need of a strong funding support from the Govt. of India. Integration of the latest computational resources into the current HPC system is the crying need of the hour.

Title of the work carried out:DFT based modelling for the Quest of Lead-free Hybrid-perovskites

Name & Designation of the Chief Investigator: Dr. Ankita Katre (DST-INSPIRE Faculty)

E-mail Id: ankita.katre@cms.unipune.ac.in

Institution Name: Centre for Modeling and Simulation, S P Pune University, Pune, India

Research Challenge/s:

The computational investigations that we carry out in materials modeling mostly deal with substantially large system size, which typically contain 300-500 atoms. Hence, in order to model these complex systems through electronic structure calculations, one always requires high performance computing facility (HPC) equipped with efficient supercomputing resources. Furthermore, depending on the nature and complexity of the properties (electronic, optical, magnetic, transport) to be determined, the required computing time is enhanced. The typical runtime for calculations of a complex atomic structure in our theoretical study is around 100 corehours.

Work carried / Milestone / Achievements:

We have recently investigated an exciting zero-dimensional lead-free hybrid-perovskite material with quantum well like structure in order to envisage the electronic structure and optical properties. Our theoretical prediction for the optical response of the hybrid perovskite system agrees well with the corresponding experimental outcome. The novel material that has been synthesized in this work is $(PD)_2Bi_2I_10.2H_2O$ or PDBI, where PD is 1,3-propanediammonium. The first principles electronic structure calculations have been carried out on Yuva-II cluster which eventually provide the deeper understanding of the electronic and optical properties of this interesting material while complementing the experimental results.

One can perceive the complexity of the crystal structure of this novel zero-dimensional perovskite materials from the following Figure 1.

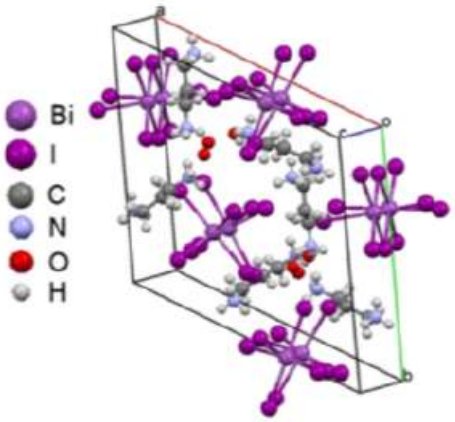


Figure.1. Unit cell of $(PD)_2Bi_2I_10.2H_2O$ (PD1,3-propanediammonium) structure.

$(PD)_2Bi_2I_10.2H_2O$ (PD1,3-propanediammonium), consists of Bi_2I_10 dimers formed by the edge sharing of BiI6 octahedra. The total number of atoms in this system is 144 (18 Carbons, 72 Hydrogens, 12 Nitrogens, 30 Iodine, 6 Bismuth and 6 Oxygen atoms).

We have performed Density Functional Theory (DFT) based electronic structure calculations to explore the optical properties of $(PD)_2Bi_2I_10.2H_2O$ (PD1,3-propanediammonium). All the ab-initio calculations for $(PD)_2Bi_2I_10.2H_2O$ are performed considering the spin polarization and with converged, fine computational parameters like energy cutoff and K-points for Brillouin Zone sampling etc. To start with, the complete structural optimization is carried out, where the lattice constants are relaxed and atomic positions are optimized. After obtaining the minimum energy configuration for this structure, we have calculated the corresponding optical absorption spectra. Along with the optical absorption spectra, we have also determined the density of states (DOS) of (PD)2Bi2I10.2H2O to estimate the band gap. The DOS calculation also facilitates the understanding of the optical absorption spectra profoundly.

Our investigation has been accepted recently in a renowned materials science journal (Impact Factor: 9.89), where I am the leading theoretical co-author, as stated below, which provides elaborative details.

Publications / Articles:

1. Zero-dimensional lead-free hybrid perovskite-like material with a quantum-well structure. JK Pious, A Katre, C Muthu, S Chakraborty, S Krishna, VC Nair, Chemistry of Materials (in press, 2019; DOI: 10.1021/acs.chemmater.8b04642).

Other ongoing works would also shape into manuscript soon.

Benefits and experience of using NPSF:

As the computing facility at NPSF is efficient, robust and extremely reliable, the complex computations required for our projects have been executed successfully without any hindrance. This is because of the proper maintenance of Yuva-II cluster by the NPSF team. Furthermore, the assistance provided by the NPSF team for installation of computational packages is also extremely appreciable.

Any other relevant information (if any):

NPSF team has always been very helpful and efficient. If asked for help regarding any simulation package or some difficulties related to the cluster, they are always very prompt in replying and keen on following-up on the problem. This efficiency of NPSF team needs to be highly acknowledged as it helps to keep the projects unaffected due to technical and computational difficulties.

Title of the work carried out: Ab initio Molecular Dynamics simulation of Ionic Liquid doped Polymer Electrolyte Membranes and Platinum Electrode Interface

Name & Designation of the Chief Investigator: Dr. Anurag Prakash Sunda
Webpage: www.apsunda.com

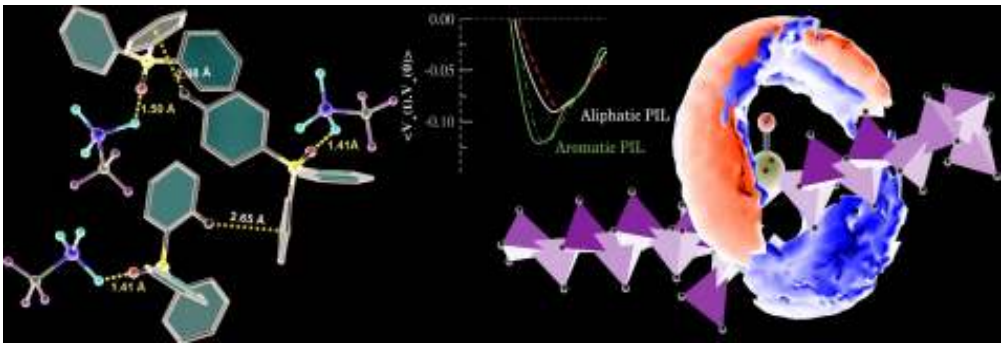
E-mail Id: anurag.sunda@gmail.com; apsunda@curaj.ac.in

Institution Name: Central University of Rajasthan

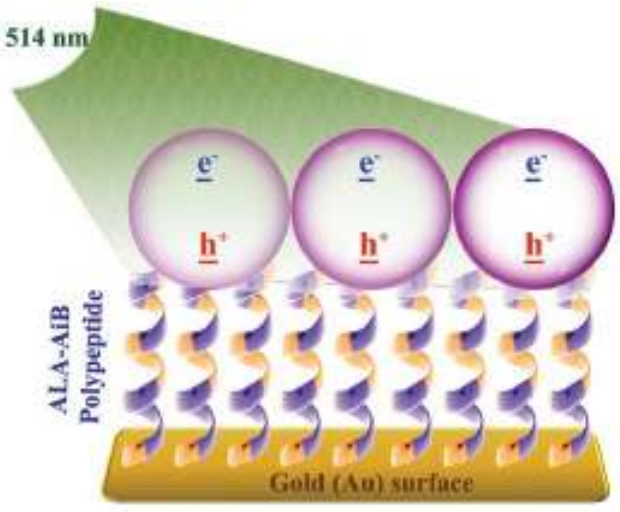
Research Challenge/s:

- Identify materials for high temperature PEM Fuel cells in anhydrous condition for Energy Applications
- Advancement in design & development of Indigenous Technology for Polymer Electrolyte Composite
- Ionic liquids for SO2/CO2 gas sequestration for environmental applications

Work carried , Milestone, Achievements & Graphs, Plots:



Mondal, A. * and Sunda, A. P.* Phys. Chem. Chem. Phys., 2018, 20, 19268-19275.



P. Roy*, N. Kantor-Uriel, and A. P. Sunda* Nanoscale, 2018, 10, 11143-11149.

Publications / Articles etc. (If any):

1. Molecular Dynamics Simulations of Ammonium/Phosphonium-based Protic Ionic Liquids: Influence of Alkyl to Aryl Group A. Mondal* and A. P. Sunda* Phys. Chem. Chem. Phys., 2018, 20, 19268-19275.

2. Nanoscale Defolding Influence of Polypeptide in Charge-Transfer Process through Organic-Inorganic Nano Hybrid System P. Roy*, N. Kantor-Uriel, and A. P. Sunda* Nanoscale, 2018, 10, 11143-11149.

Awards (If any):

Best Poster Award in Theoretical Chemistry Symposium (TCS) 2019

Work presented in conference/s with photographs (if any):

- Theoretical Chemistry Symposium (TCS) 2019 held at BITS-Pilani

Appreciation / Recognition (if any):

References:

Benefits experience of using NPSF:

I could able to do progress in my Research Project and NPSF support help to complete my calculations using parallel run.

Any other relevant information (if any):

Title of the work carried out: First-Principle Study of the Electronic Structures of Heterostructure Devices and Their Related Applications.

Name & Designation of the Chief Investigator: Dr. Anver Aziz (Assistant Professor)

E-mail Id: aaziz@jmi.ac.in

Institution Name: Jamia Millia Islamia, New Delhi

Collaborator :

Dr. Bhalchandra Pujari (Assistant Professor), Center for simulation and Modelling, Savitribai Phule Pune University

Research Challenge/s:

We have successfully performed calculations for gas sensors and FETs and also studying the heterostructures for the applications of Schottky and Ohmic contacts.

Work carried , Milestone, Achievements & Graphs, Plots:

All plots and graphs related to publications are attached with the work presented in the section given below.

Publications / Articles etc. (If any):

Two papers have been accepted for publication in the AIP conference proceeding given in the section below.

Awards (If any):

CSIR-SRF awarded to Mr. Mohammad Ubaid on the basis of this work.

Work presented in conference/s with photographs (if any)

1. Presented (ORAL) a paper entitled "Adsorption of Na atom on Mono-Layer Gallenene" in an International Workshop on Material for Energy Applications, December 6-9, 2018, S.S Jain Subodh P.G. (Autonomous) College, Jaipur, Rajasthan, India.

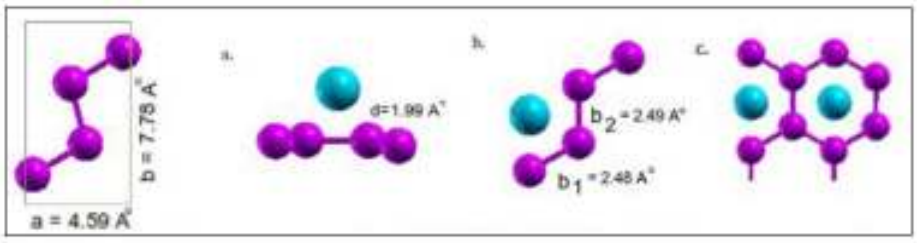


Fig.1. Top (a) and side (b) view of Na adsorbed mono-layer Ga 100 and the top (c) view of 2x2 Na adsorbed mono-layer Ga 100 .

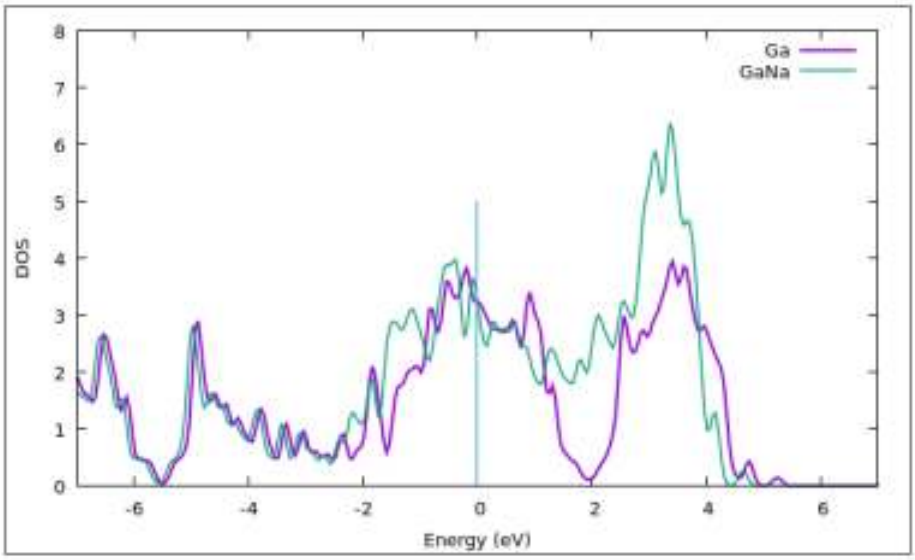


Fig. 2. Electronic density of states of pristine and Na adsorbed Ga100 (a) and of Na-Ga100 where EF is set to zero.

2. Presented (POSTER) a paper entitled "First Principle Study of In/Ga-Doped Phosphorene" in 63^{rd} DAE Solid State Physics Symposium, December 18-22, 2018, GJU of Science and Technology, Hisar, Haryana. Organized by: BARC, Mumbai.

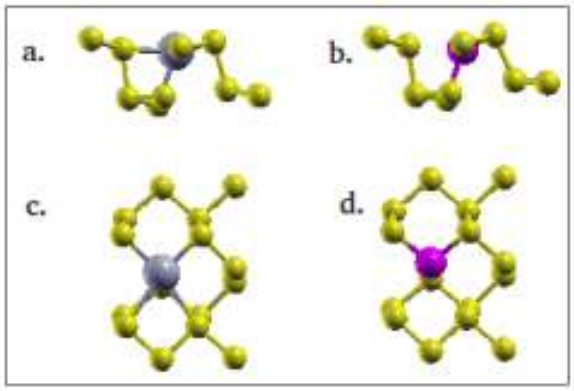


Fig. 1. Side (a,b) and Top (c,d) views of In (a,c) and Ga (b,d)doped 2x2 phosphorene supercells.

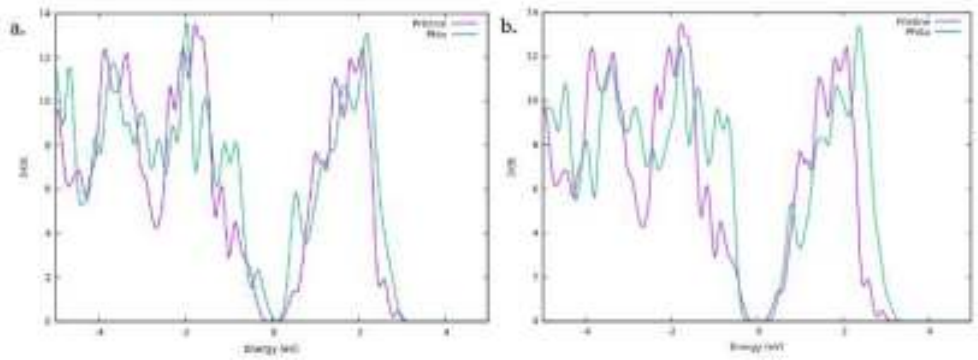


Fig. 2. Density of states of In (a) and Ga (b) doped phosphorene, where EF is set to zero.

Appreciation / Recognition (if any):

Work presented for poster at Jaipur conference was upgraded by organizers to oral presentation.

References:

1. Geim, A. K.; Novoselov, K. S. Nat. Mater. 2007, 683191.doi:10.1038/nmat1849 .
2. S. Grimme et al, J. Chem. Phys 132, 154104 (2010).
3. Giannozzi, P. et al. QUANTUM ESPRESSO: a modular and open-source software project for quantum simulations of materials. J. Phys. Condens. Matter 21, 395502 (2009) .

Benefits & experience of using NPSF:

Our experience of using NPSF is great. Due to NPSF, we are able to do expensive calculations in a very short time. We wish to thank National NPSF for providing the computation facility by PARAM Yuva II cluster.

Any other relevant information (if any):

It is very difficult to carry out some phonon calculations because the given wall time (maximum 7 days) is not sufficient. We request you to give some extra time to counter these type of expensive calculations.

Title of the work carried out: Probing translational and rotational dynamics in hydrophilic/hydrophobic anion based imidazolium ionic liquidwater mixtures

Name & Designation of the Chief Investigator: Dr. Arun Venkatnathan, Associate Professor

E-mail Id: arun@iiserpune.ac.in

Institution Name: Indian Institute of Science Education and Research, Pune

Research Challenge/s: Molecular Simulation of Ionic Liquids require long simulation times to observe certain properties. (e.g. rotational motions)

Work carried , Milestone, Achievements & Graphs, Plots:

In this work, we examine the effect of water concentration and temperature on the dynamical properties of [Hmim][Cl] and [Hmim][NTf_2] Ionic Liquids (ILs). The dynamical properties such as translational diffusion coefficients, ion-pair lifetimes, and rotational correlation times are calculated using Molecular Dynamics simulations. The simulations predict that water concentration also significantly impacts the magnitude of dynamical properties. At low, intermediate and high water concentrations, the following trend in diffusion coefficients is seen: Cl^- > $Hmim^+$; Cl^- > $NTf_2{}^-$; $Hmim^+$ ([Hmim][Cl]) > Hmim+ ([Hmim] [NTf_2]). At ultra-low water concentrations of [Hmim][Cl] IL, several bridge like configurations form between water molecules and Cl^- anions, which are supported by a complex distribution of water clusters. The effect of an increase in the water concentration leads to a decrease in ion-pair lifetimes between the $Hmim^+$ cations and Cl^-/$NTf_2{}^-$ anions, which strongly correlate with the trends observed from the diffusion coefficients. A biexponential function was found to be the best fit for the RACF at neat/ultra-low water concentrations of [Hmim][Cl] and [Hmim][NTf_2] ILs, whereas a single exponential function was sufficient to fit the RACF at low, intermediate and high water concentrations. The rotational relaxation time of the Hmim+ cations is larger in neat [Hmim][Cl] compared to that in neat [Hmim][NTf_2] with an opposite trend seen with hydration. The rotational correlation time of water molecules is larger in [Hmim][Cl] compared to that in [Hmim][NTf_2] at low and intermediate water concentrations, with similar correlation times observed at high water concentrations.

Publications / Articles etc. (If any):

P. Kumar, P. Prakash, K. R. Ramya and **A. Venkatnathan**, Probing Translational and Rotational Dynamics in Hydrophilic/Hydrophobic Anions based Imidazolium Ionic Liquid-water mixtures Soft Matter, 14, 6109 (2018)

Awards (If any): -
Work presented in conference/s with photographs (if any):-
Appreciation / Recognition (if any):-
References:-
Benefits & experience of using NPSF:-
Any other relevant information (if any):-

Title of the work carried out: Design, Synthesis and Evaluation of Modified Short Peptides as Inhibitors of Amyloid-β (Aβ) Peptide Aggregation.

Name & Designation of the Chief Investigator: Deepti Goyal (Ph.D.), Assistant Professor

E-mail Id: deepti.bansal.chem@gmail.com; deeptig@iitbombay.org

Institution Name: Sri Guru Granth Sahib World University, Fatehgarh Sahib, Punjab.

Research Challenge/s:

1. To rationally design and synthesize novel molecular frameworks.
2. To evaluate the inhibitory activity of the synthesised compounds towards Aβ peptide aggregation by using various techniques such as Fluorescence spectroscopy, Atomic Force Microscopy (AFM), NMR (1D and 2D), Circular Dichroism etc.
3. To understand the molecular mechanism behind the inhibitory activity of the synthesised compounds towards A peptide aggregation by computational methods.

Work carried , Milestone, Achievements & Graphs, Plots:

Amyloid-β (Aβ) peptide instinctively aggregate and form plaques in the brain of Alzheimer's disease (AD) patients. At present, there is no cure or treatment for AD, and significant effort has, therefore, been made to discover potent drugs against AD. Previous studies reported that a resveratrol and clioquinol hybrid compound ((E)-5-(4-hydroxystyryl)quinolone-8-ol), C1, strongly inhibit Aβ_{42} aggregation and disassemble preformed fibrils. However, the atomic level details of the inhibitory mechanism of C1 against Aβ_{42} aggregation and protrofibril disassembly remains elusive. In this regard, molecular docking and molecular dynamics (MD) simulation of Aβ_{42} monomer, Aβ_{42} monomer C1 complex, Aβ_{42} protofibril, and Aβ_{42} protofibril C1 complex were performed in the present study. MD simulations highlighted that C1 bind in the central hydrophobic core (CHC) region, i.e., KLVFF (16-20) of Aβ_{42} monomer, which play a critical role in Aβ_{42} aggregation. C1 promote the formation of native helical conformation in the Aβ_{42} monomer and decrease the probability of D23-K28 salt bridge interaction that is critical in the formation of aggregation-prone βsheet conformation. Further, C1 destabilize Aβ_{42} protofibril structure by increasing the interchain distance between chains AB, disrupting the saltbridge interaction between D23-K28, and decreasing the number of backbone hydrogen bonds between chains AB of the Aβ_{42} protofibril structure. The insights into the underlying inhibitory mechanism of small molecules that display potential in vitro anti-aggregation activity against Aβ_{42} will be beneficial for the rational design of more potent drug molecules against AD.1

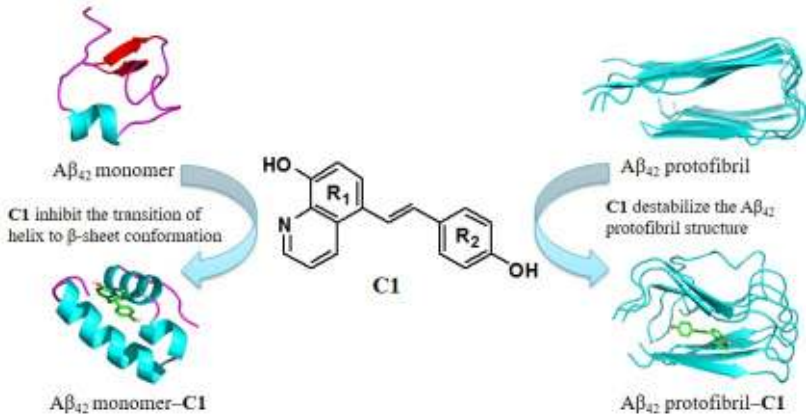


Figure 1:Pictorial representation of the inhibitory mechanism of C1 against Aβ_{42} aggregation and protrofibril disassembly.

The aggregation of amyloid-β peptide (Aβ) has been associated with the pathogenesis of Alzheimers disease (AD). The recent studies highlighted that L17A/F19A double mutation increases the structural stability of Aβ_{40} and diminish Aβ_{40} aggregation. However, the underlying effect of L17A/F19A double mutation on the Aβ_{40} structure and dynamics remain elusive. In this regard, the influence of L17A/F19A double mutation on the structure and dynamics of Aβ_{40} was investigated using all-atom molecular dynamics simulation. MD simulation reveal that mechanism behind modulation of Aβ_{40} aggregation is associated with decrease in the βsheet content and dynamics of the salt bridge D23-K28. The secondary structure analysis highlight more abundant -helix content in the central hydrophobic core (CHC) and C-terminal region of Aβ_{40} upon L17A/F19A double mutation that is consistent with CD results. The free energy landscape (FEL) reveal that coil conformation is the most dominant conformation in Aβ_{40} whereas the helical conformation is the most-populated and energetically favourable conformation in Aβ_{40}(L17A/F19A). MD simulation, in accord with the experiment, highlight that L17A/F19A double mutation diminish Aβ_{40} aggregation as the population of the fibril-prone state substantially decreased. The present study, in conjunction with experiment, highlight that L17 and F19 are the critical residues involved in the conformational change that trigger neurotoxic cascade of Aβ_{40}. Overall, MD simulation provide key structural and physical insights into the reduced Aβ_{40} aggregation upon L17A/F19A double mutation and an atomic picture of the L17A/F19A-mediated conformational changes in Aβ_{40}.2

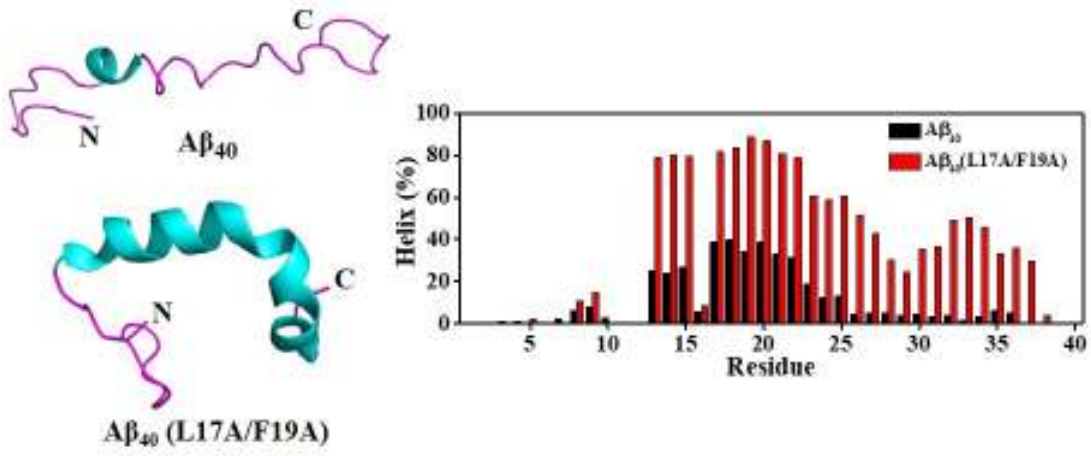


Figure 2:Pictorial representation of the influence of L17A/F19A double mutation on the structure and dynamics of Aβ_{40}.

Publications / Articles etc. (If any):

1. Molecular Insights into the Effect L17A/F19A Double Mutation on the Structure and Dynamics of Aβ_{40}: A Molecular Dynamics Simulation Study. R. K. Sani, S. Shuaib, D. Goyal, B. Goyal J. Cell. Biochem. 2018, 119, 8949.

2. Assessing the Effect of D59P Mutation in the DE Loop Region in Amyloid Aggregation Propensity of 2-Microglobulin: A Molecular Dynamics Simulation Study. S. S. Narang, S. Shuaib, D. Goyal, B. Goyal J. Cell. Biochem. 2018, 119, 782.

3. Insights into the Inhibitory Mechanism of a Resveratrol and Clioquinol Hybrid against Aβ_{42} Aggregation and Protofibril Destabilization: A Molecular Dynamics Simulation Study. R. K. Sani, S. Shuaib, D. Goyal, B. Goyal J. Biomol. Struct. Dyn. 2018, 1.

Awards (If any): NIL

Work presented in conference/s with photographs (if any)

1. International conference-cum-workshop on Informatics Tools in Drug Discovery and Drug Delivery from 1-4 November, 2018 at Punjabi University, Patiala.

2. 11th National Conference on Recent Trends in Chemical and Environmental Sciences from 7-8 February, 2019 organised by Department of Chemistry, Punjabi University, Patiala.

Appreciation / Recognition (if any): NIL

References:

1. R. K. Sani, S. Shuaib, D. Goyal, B. Goyal, Insights into the Inhibitory Mechanism of a Resveratrol and Clioquinol Hybrid against Aβ_{42} Aggregation and Protofibril Destabilization: A Molecular Dynamics Simulation Study. J. Biomol. Struct. Dyn. 2018, 1.

2. R. K. Sani, S. Shuaib, D. Goyal, B. Goyal, Molecular Insights into the Effect L17A/F19A Double Mutation on the Structure and Dynamics of Aβ_{40}: A Molecular Dynamics Simulation Study. J. Cell. Biochem. 2018, 119, 8949.

Benefits & experience of using NPSF:

The computational facility provided by CDAC is of great support to the Ph.D. students and M.Sc. students to pursue their research projects and timely completion of research work. The benefit of the NPSF is that the simulations can be completed in short time. The NPSF facility is easy to access and the staff at CDAC is very cooperative and quickly response to our queries. We thank the entire team of NPSF for their extended support and cooperation.

Any other relevant information (if any): NIL

Title of the work carried out: Strain Induced Tunable Schottky Barriers in Borophene/MX2 Van der Waals Heterostructures

Name & Designation of the Chief Investigator: Dr. Jagdish Kumar

E-mail Id: nehakatoch2@gmail.com

Institution Name: Central University of Himachal Pradesh

Research Challenge/s:

To study Noble 2D Materials based Heterostructures for Nanoelectronics applications using First Principle Methods.

Work carried , Milestone, Achievements & Graphs, Plots:

We have studied systematically the strain dependent tuning of electronic properties for 12 borophene/MX2 (M = Mo, W and X = S, Se) vdW Heterostructures within the framework of Density Functional Theory as implemented in VASP code. We have applied in-plane uniaxial compression (expansion) strain and biaxial compression (expansion) strain respectively. Results have shown the transformation of schottky barriers into ohmic contacts between the heterointerface of borophene/MX2 heterostrcutures in all compression strains and biaxial expansion in borophene/MoS2 which can be used to fabricate high performance nanoelectronic devices. We have also studied the effect of vertical pressure on the Schottky barrier heights (SBHs). In addition, we have calculated electron transport properties of borophene/MX2 heterostrcutures which confirm the transformation of schottky barriers into ohmic contacts on compression strains.

Publications / Articles etc. (If any):

Manuscript is ready for submission.

Awards (If any): No

Work presented in conference/s with photographs (if any): No

Appreciation / Recognition (if any): No

References:

Benefits & experience of using NPSF:

It's a nice experience of using NPSF, quick response of querries and helping towards installations.

Any other relevant information (if any): No

Title of the work carried out:

1. Thermoelectric Properties of Cs2InXCl6 (X=Sb, Bi) : A First Principles Study
2. Thermoelectric performance of cost-effective cubic perovskites: Cs2SnI6
3. Thermoelectric Properties of Cs2TiBr6 : A First Principles Study

Name & Designation of the Chief Investigator: Dr. K.C. Bhamu

E-mail Id: kc.bhamu@ncl.res.in

Institution Name: CSIR-NCL, Pune

Research Challenge/s:

I love to use Wien2k for my projects which deals the jobs in three different ways: (I) k-point parallelization (ii) mpi-parallelization and (iii) hybrid jobs. For small systems the k-point parallelization is good but for the complex jobs (my main objective of the project) it is tough to deal Wien2k. Also, Wien2k is full potential code so it takes more time to execute the jobs than other DFT codes like QE/VASP. So the main challenges are: Getting mpi and mpi+k-point parallelization job script for wien2k. (2) Queue time is much long for small jobs which some times frustrates. So I would like to request C-DAC team to reduce the queue time for small jobs and make a mpi and mpi+k-point parallelization job scripts so that the complex jobs can also be done effectively and efficiently. Some example scripts can be seen from here:
`http://www.nersc.gov/users/software/applications/materials-science/wien2k/`

Work carried , Milestone, Achievements & Graphs, Plots: The work is not published yet.

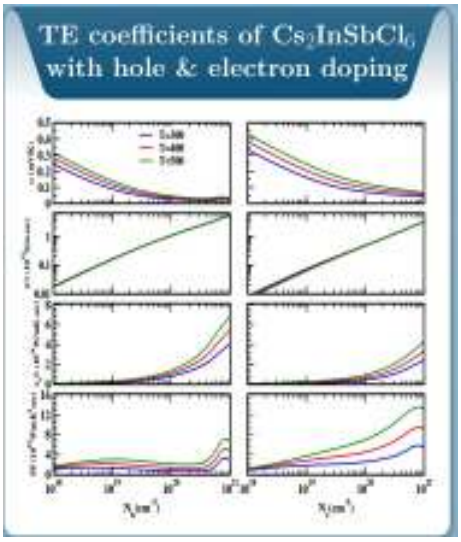
Publications / Articles etc. (If any): NA (under writing process).

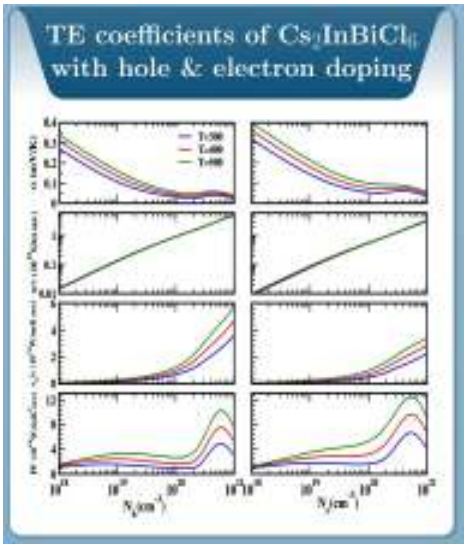
Awards (If any):

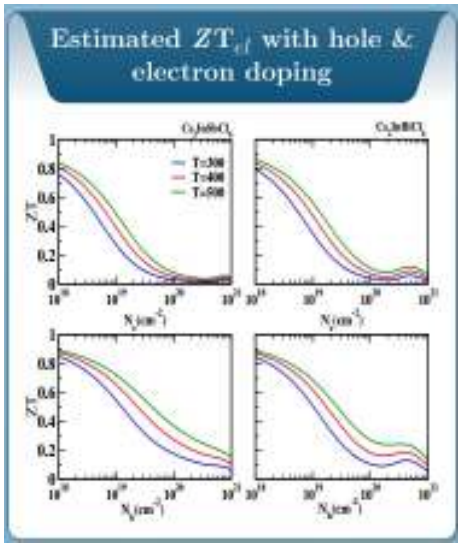
1. Best Oral presentation award for the work entitled Thermoelectric performance of cost-effective cubic perovskites: Cs2SnI6 presented in the International Conference on Recent Trends in Environment Sustainable Development (RTESD-2018) organised by Vivekananda Global University Jaipur during 23-25 Feb., 2018.
2. Best Poster presentation award for the work entitled Thermoelectric Properties of Cs2InXCl6 (X=Sb, Bi) : A First Principles Study presented in the International Conference on Recent trends in Environment & Natural Sciences ICRTENS-2019 organized by Govt. Science College, Sikar Rajasthan during 12-13 Feb., 2019.

Work presented in conference/s with photographs (if any):

Using NPSF-CDAC facilities, I have performed various DFT calculations. Below are some photographs:







Appreciation / Recognition (if any):

Won two awards in International Conferences.

References:

Benefits & experience of using NPSF:

For the successful compilation of my project I could finish some important jobs using NPSF facilities which was possible because of good technical support from C-DAC team.

Any other relevant information (if any):

CDAC, Pune has been doing a wonderful job for many years in helping Computational Scientists in their active pursuit of research, across India. The strong computational support provided by CDAC-Pune enables us to pursue good quality research. The numbers of nodes are not enough to run the calculation in less queue time therefore. I would like to draw attention of Indian Government to provide enough financial support to NPSF-C-DAC so that the latest Computational facilities can be provided to users by C-DAC.

Title of the work carried out: Diversity and functionality of small dsRNA produced by food fermenting lactic acid bacteria

Name & Designation of the Chief Investigator: K. Jeyaram, Scientist-D

E-mail Id: jeyaram.ibsd@nic.in

Institution Name: Institute of Bioresources and Sustainable Development (IBSD)

Research Challenge/s:

Insilco target prediction of small double-stranded RNA (isolated from food fermenting Lactic acid bacteria) on human transcriptome an HIV transcriptome using bioinformatics algorithms PITA, TargetScan and miRanda.

Work carried, Milestone, Achievements & Graphs, Plots:

The sequence of millions of dsRNA produced by lactic acid bacteria were subjected to in-silico target prediction. Promising target on pathways leads to anti-inflammatory, anticancer and antiviral properties were predicted. At present, we are validating the predicted activity in cell lines in collaboration with C-CAMP Bangalore and NIRRH (ICMR), Mumbai. An example of the results obtained by the in-silco target prediction using NPSF is shown in Fig. 1 (Enclosed).

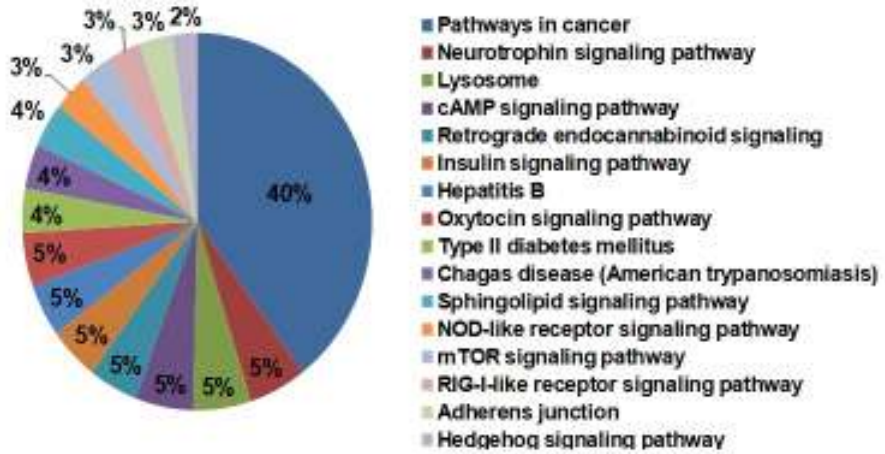


Fig. 1 The results of *Insilco* target prediction using NPSF shows the major pathways targeted by the small dsRNA produced by *Lactobacillus plantarum* (a food fermenting bacteria).

Publications / Articles etc. (If any): Nil

Awards (If any): Nil **Work presented in conference/s with photographs (if any):** Nil

Appreciation / Recognition (if any): Nil

References: Nil

Benefits & experience of using NPSF:

We could handle millions of dsRNA sequences against thousands of human transcriptome sequences in a very shorter period of 2 months. We thank NPSF for allowing such a facility for us.

Any other relevant information (if any): Nil

Title of the work carried out: Classical Chemical Dynamics Simulations: Reaction Dynamics and Mechanisms

Name & Designation of the Chief Investigator: Dr. Manikandan Paranjothy, Assistant Professor

E-mail Id: pmanikandan@iitj.ac.in

Institution Name: Indian Institute of Technology Jodhpur

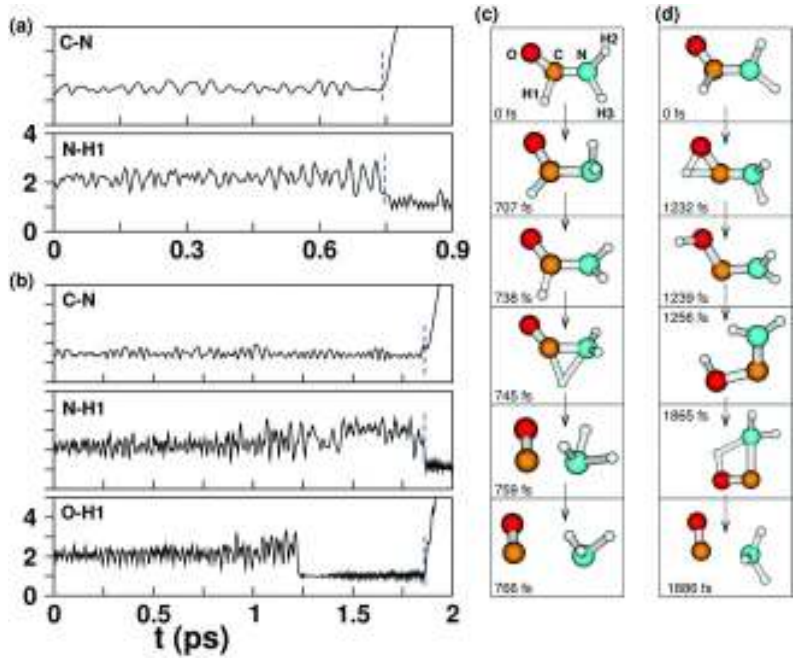
Research Challenge/s:

The technology we use in our research group is called Direct Dynamics Simulations which we employ to study organic reaction mechanisms, decomposition pathways, branching ratios, etc, for interesting chemical and biochemical reactions. This technique requires integration of Newtons equations of motion and the required potentials and forces for the integration are computed on-the-fly using a chosen level of electronic structure theory (quantum chemistry). In general, one requires to generate atleast 100 classical trajectories in a simulation. Assuming integration to be carried out till 3 picosecond (3000 femtosecond) and an integration step size of 1 femtosecond, we need to perform 3000 single point electronic structure calculations for one trajectory. For 100 trajectories, we need to perform 3000*100 = 300000 single point electronic structure calculations. Please note that the values reported here are bare minimum requirements for classical trajectory simulations and only with increase in number of trajectories, the accuracy of the results improve. To carry out such an enormous amount of calculations, we utilize the CDAC PARAM Yuva II facility. The kind of computational power required is not available in the institute where the PI is associated with.

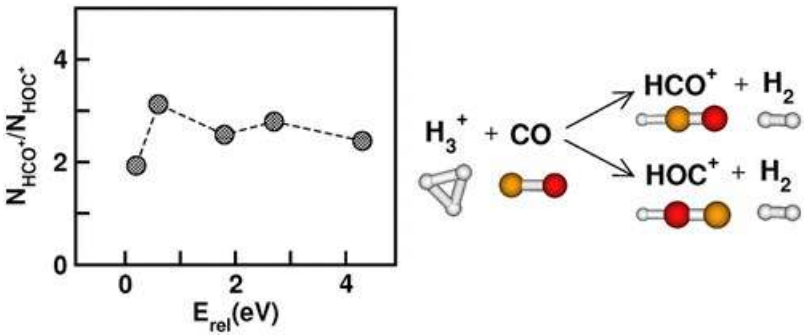
Work carried , Milestone, Achievements & Graphs, Plots:

Between the period January 01, 2018 to December 31, 2018, we utilized the NPSF facility to carry out direct dynamics simulations on the following projects: (1) Unimolecular decomposition of formamide which contains 6 atoms (24 electrons), (2) bimolecular collision dynamics of H_3^+ + CO system (16 electrons) and (3) dissociation pathways of halons (more than 60 electrons). A brief summary of these works is given below:

1. Unimolecular decomposition of formamide: Formamide (NH_2CHO), being the simplest organic molecule containing an amide functional group, serves as a prototype to study protein and peptide chemistry. Formamide has been found in Comets and interstellar media and its decomposition results in smaller molecules such as NH_3, CO, HCN, HNCO, etc. These smaller molecules are considered to have been potential precursors for the formation of complex biological molecules, such as nucleic acids and nucleobases, in the early Earth. Several experimental and theoretical investigations of formamide decomposition have been reported in the literature. Unimolecular decomposition of formamide in the electronic ground state was investigated by classical direct chemical dynamics simulations. The calculations were performed at three different energies using the density functional B3LYP/aug-cc-pVDZ level of electronic structure theory. The major dissociation products observed were NH_3, CO, H_2, HNCO, H_2O, HCN, and HNC along with products of a few minor dissociation channels. Reactivity, atomic level mechanisms, and product branching ratios were investigated as a function of total energy.



2. Bimolecular collision dynamics of H_3^+ + CO reaction: The proton transfer reaction H_3^+ + CO $HCO^+/HOC^+ + H_2$ has gained considerable attention in the literature due to its importance in interstellar chemistry. The reaction products - formyl cation (HCO^+) and isoformyl cation (HOC^+) - are known to initiate multiple chemical reaction networks, resulting in complex molecules found in space. Several experimental and theoretical studies probing the structure and energetics of the $[H_3CO]+$ system, HCO^+/HOC^+ product branching ratios, reaction mechanisms, etc., have been reported in the literature. In the present work, we investigated the H_3^+ + CO bimolecular reaction in the gas phase using direct dynamics methodology. The simulation conditions were chosen to mimic recently reported velocity map imaging experiments on the same reaction. The calculations were performed using the density functional PBE0/aug-cc-pVDZ level of electronic structure theory. Internal energy and scattering angle distributions of reaction products found from the simulations are in qualitative agreement with the experiment. However, the product branching ratios at low collision energies were in contrast with the experimental predictions. Interesting dynamical features were observed in the simulations, and detailed atomic level mechanisms are presented.



3. Dissociation dynamics of Halons: Decomposition chemistry of Halons has received much attention due to their role in ozone depletion. An important aspect of dissociation of halons is the competition between radical and molecular pathways. Recently, role of isomerization in the molecular pathways were studied using electronic structure theory. In the present work, we investigate the dissociation chemistry of CF_2C_l2, CF2Br_2, $CHBr_3$, and CH_2BrCl using chemical dynamics simulations. Classical trajectories were generated on-the-fly at the

density functional PBE0/6-31G* level of electronic structure theory at a fixed total energy. Simulations showed that molecular products, in general, were dominant for all the four molecules at the chosen energy. A variety of reaction mechanisms including isomerizations and roaming pathways contributed to the formation of molecular products.

Publications / Articles etc. (If any):

1. Unimolecular decomposition of formamide via direct chemical dynamics simulations, A. Gahlaut and M. Paranjothy, Phys. Chem. Chem. Phys. 2018, 20, 8498 - 8505 (DOI: 10.1039/c8cp00541a).

2. Direct chemical dynamics simulations of H_3^+ + CO bimolecular reaction, E. G. Naz, S. Godara and M. Paranjothy, J. Phys. Chem. A 2018, 122, 8497 - 8504 (DOI: 10.1021/acs.jpca.8b08671).

Awards (If any):

Work presented in conference/s with photographs (if any):

The work discussed here were presented in the following conferences by students associated with the projects.

1. **Spectroscopy and Dynamics of Molecules and Clusters 2018**, February 15-18, 2018, organized by IISER Kolkata.

2. **Nothwest Meeting on Spectroscopy, Structure and Dynamics**, March 16-18, 2018, organized by MNIT, Jaipur.

Appreciation / Recognition (if any):

References:

Benefits & experience of using NPSF:

As mentioned above, our simulations are memory and processor intensive which we could smoothly carry out in the NPSF facility. Many different compilers are available in the facility and we could select the right compiler for our codes. We definitely look forward to using the facility continuously.

Any other relevant information (if any):

Title of the work carried out: Photovoltaic-App-PR (Simulations of rare earth free permanent magnetic materials and inorganic halide perovskites for photovoltaic applications)

Name & Designation of the Chief Investigator: Dr. Manish K. Kashyap

E-mail Id: mkumar@kuk.ac.in

Institution Name: Kurukshetra University, Kurukshetra

Research Challenge/s:

The proposed work has been planned with the following objectives:

1. To produce downshift/upshift in the band gap by proper doping, disorders and alloying in halide perovskites so that the resultant material may lie in optimal region and can be used for photovoltaic applications.
2. Tuning optical properties of halide perovskite by varying chemical composition.
3. To find accurate band structures of halide perovskites using orbital independent mBJLDA XC potentials in order to simulate actual experimental facts.
4. To analyze absorption spectra, refractive index and dielectric function response of halide perovskites with energy range useful for photovoltaic applications.
5. To search novel and fantastic hard magnetic materials based on alloys formation with Fe, Co and Mn as main element.
6. To explore the magnetic anisotropy in new advanced magnetic materials induced by interstitial/ substitutional doping by B, C etc.
7. To calculate the electronic structure of RE free magnetic materials using Coulomb corrected GGA (GGA+U) functional to account for accurate exchange and correlation effects.

Work carried, Milestone, Achievements & Graphs, Plots:

The increasing consumption but restricted resources of fossil fuels and issuance of greenhouse gases or current pollution levels in metropolitan areas are forcing researchers to search for new, clean and renewable prospective energy resources. The benefits of renewable energy are environmental-amicability, sustainability and domestic energy security [1,2]. Today permanent magnets (PMs) are being used in various clean energy applications ranging from electronics, mechanics, transportation to power generations [3-5]. The important properties of a PM include its coercivity (Hc), magnetization (Ms) and maximum energy product ((BH)max). A high (BH)max is a necessary, but not a sufficient condition for a commercially viable PMs. In addition to optimum value of Ms, a permanent magnetic material must also have a sufficient value of Hc in order to resist demagnetization under maximum load and temperatures so that it remains stable enough for applications over expected lifetime. Coercivity is a consequence of magnetocrystalline anisotropy (MCA) which originates due to spin-orbit coupling (SOC) along a particular direction. The PMs composed of critical RE (Nd, Sm and Dy) and transition-metal (TM) elements have

largest MCA value e.g. Nd2Fe14B is champion magnet that has MCA value of ∼ 5 MJ/m3 [6] which is due to strong 3d-4f SOC effect. A high risk of unavailability and large price of these critical RE elements attracted attention to look for development of new high performance novel RE free permanent magnets [7,8] that can be used in clean energy applications such as wind turbines and electric vehicles. In this regard, we have studied novel materials that have great potential to use as rare earth (RE) free permanent magnetic materials under the framework of density functional theory (DFT) [9]. And we mainly used the PAW method as implemented in the VASP package [10] and FPLAPW calculations as implemented in WIEN2k code [11].

Among possible materials for replacing RE elements in PMs, the ordered L10-FeNi [12-15] is the one, with extraordinary magnetic response viz (i) a large theoretically possible (BH)max of ∼ 446 kJ/m3 due to its large saturation magnetization (Ms) of ∼ 1.5 T, (ii) a Curie temperature of at least 830 K which is sufficiently larger than that of Nd2Fe14B ∼ 590 K, and (iii) optimum value of experimentally measured MCA which oscillates around 1.0 MJ/m3, depending on the manufacturing techniques used. But even such high value is insufficient for PMs. However, there is still a scope to improve its MCA by certain modifications like introducing tetragonal strain, with interstitial doping or by substitutional alloying. In order to promote structural stability and tune MCA of L10-FeNi, it is tetragonally distorted by introducing an interstitial C/N-doping.

N-doped L10-FeNi:
For that one N-atom added in interstitial site of four Ni/Fe atoms in a 221 supercell (Fig.1).

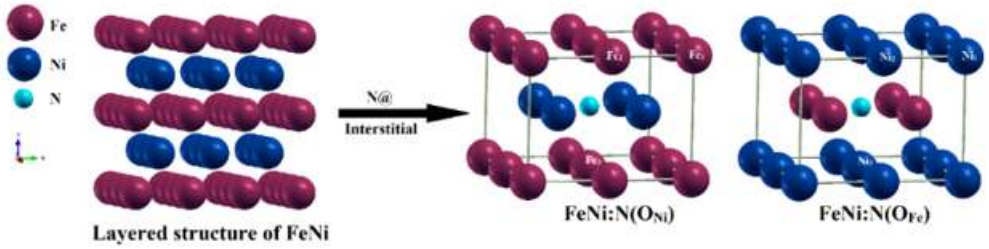


Fig. 1. Schematics of the 2×2×1 supercell of FeNi with two different kind of N-doping. FeNi:N(O_{Ni})/FeNi:N (O_{Fe}) represents N doping at interstitial sites in Fe/Ni-layer.

TABLE 1. Optimized lattice parameters (in Å) and formation energy (E_{For}) (in eV) of pristine and FeNi:N compounds

Compound	Lattice Parameters		c/a	E_{For}
	A	c		
FeNi	2.531	3.579	1.414	-0.18
FeNi:N(O_{Fe})	2.554	3.778	1.479	-2.26
FeNi:N(O_{Ni})	2.561	3.714	1.450	-2.35

Our calculated DOS predicts that FeNi is spin polarized while on addition of N, some states get accommodated near the Fermi level (EF) in majority spin channel of FeNi:N which reduces its spin polarization (Fig. 2). In FeNi:N(ONi/OFe), due to asymmetry caused by interstitial N-impurity, all Fe/Ni atoms can be categorized as three non-equivalent atoms as mentioned by Fe1, Fe2 and Fe3/Ni1, Ni2 and Ni3. The DOS in the vicinity of EF are due to the admixture of Fe3-3d/Ni3-3d and N-2p states.

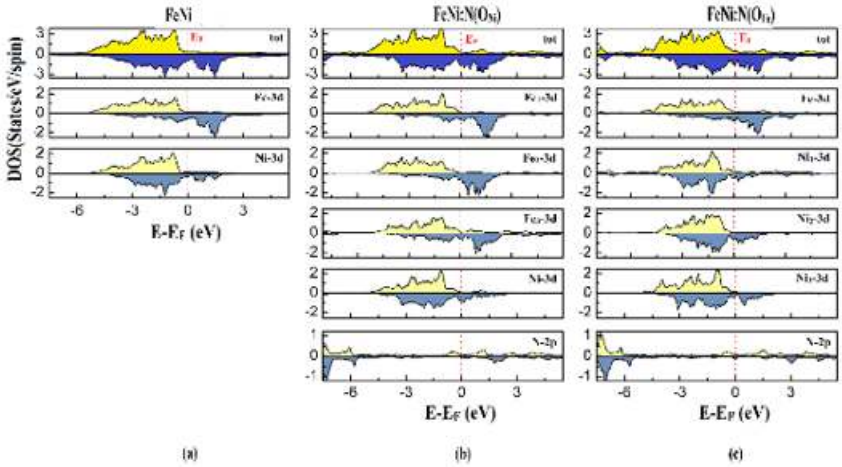


Fig. 2. Calculated total and orbital projected DOS of (a) FeNi (b) FeNi:N(O_{Ni}) and (c) FeNi:N(O_{Fe}) compounds. Fermi level (E_F) is shifted to 0 eV

TABLE 2. Calculated total and atom resolved spin magnetic moments (μ_s), orbital magnetic moments (μ_l), magnetization (M_s) and MCA (K) in of FeNi and FeNi:N compounds

Compound	Direction		Magnetic Moments (μ_B)						M_s (T)	K (MJ/m^3)
			Fe			Ni		Total		
FeNi	001	μ_s	2.701			0.645		3.271	1.67	0.43
		μ_l	0.054			0.036				
	100	μ_s	2.702			0.645		3.271		
		μ_l	0.049			0.038				
	Expt.	μ_s	2.540[16]			0.730[16]			1.47[14]	0.58-1.3[13-15]
		μ_l	0.050[17]			0.100[17]				
FeNi:N(O_{Ni})			Fe_1	Fe_2	Fe_3	Ni	N	Total		
	001	μ_s	2.740	2.895	2.037	0.579	0.059	3.226	1.53	0.95
		μ_l	0.063	0.059	0.042	0.036	0.001	-		
	100	μ_s	2.741	2.895	2.038	0.580	0.060	3.229		
		μ_l	0.048	0.046	0.007	0.030	0.002	-		
FeNi:N(O_{Fe})			Fe	Ni_1	Ni_2	Ni_3	N	Total		
	001	μ_s	2.394	0.346	0.861	0.847	-	3.043	1.46	0.63
		μ_l	0.047	0.024	0.054	0.053	0.046 0.004	-		
	100	μ_s	2.392	0.346	0.860	0.847	-	3.041		
		μ_l	0.041	0.007	0.054	0.051	0.045 0.002	-		

The total spin magnetic moment of FeNi:N(ONi/OFe) decreases due to the hybridization of Fe3-3dNi-3d/Fe-3dNi3-3d with non-magnetic impurity atom, N-2p. This decrease is more in FeNi:N(OFe) due to antiparallel arrangement of N-2p states with Fe-3d states and Ni-3d states. The calculated spin magnetic moments are isotropic for all the compounds. However, orbital magnetic moments are directional dependent and orbital moment anisotropy (OMA) defined by $\Delta\mu_{orb}=\mu_{orb}^{([001])}-\mu_{orb}^{([100])}$ is found as 0.005 B for Fe and -0.002 B for Ni in pristine FeNi. This observation is in good agreement with Miuara et al. [19]. In case of FeNi:N(ONi), the observed OMA is 0.021/0.006/-0.001 B for Fe/Ni/N and in FeNi:N(OFe), this value is 0.006/0.006/0.002 B. Hence, the overall sum of OMA increases in both cases.

On interstitial N-doping, Ms decreases from 1.67 T to 1.53/1.46 T for FeNi:N(ONi/OFe) case (Table 2). This decrease is larger in FeNi:N(OFe) due to decrease in Fe moment which

exists in the plane containing non-magnetic N impurity. Further, Fe is anti-ferromagnetically coupled with N impurity in this situation. The calculated MCA of L10-FeNi is 0.43 MJ/m3 that is comparable to 0.47 MJ/m3 as calculated by Werwinski et al. [18] However, its experimentally measured value oscillates around 1 MJ/m3 [13-15] depending on the synthesis technique used. On addition of interstitial N-doping, the MCA increases to 0.95/0.63 MJ/m3 for FeNi:N(ONi/OFe). This increase may be attributed to the tetragonal distortion i.e. increased c/a ratio. The similar observations were also noticed by Miuara et al. [19] and Manchanda et al. [20] for pristine FeNi and FeNi:B case, respectively. Further, the anisotropy energy per atom is directly proportional to OMA i.e. larger OMA results large MCA. In FeNi:N, enhancement in OMA gives large MCA. Moreover, in FeNi:N(ONi) orbital anisotropy is even larger that allows larger MCA (0.95 MJ/m3) than FeNi:N(OFe) (0.63 MJ/m3).

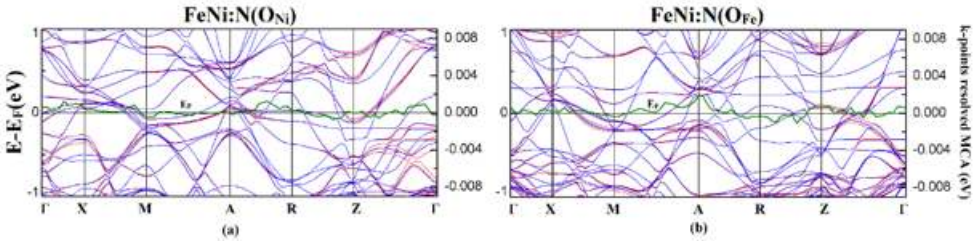


Fig 3. Band structure including SOC with magnetization along [100] (blue lines) and [001] directions (red lines) along with the MCA contribution per k-point (green) for (a) FeNi:N(O$_{Ni}$) (b) FeNi:N(O$_{Fe}$).

In order to find the origin of the MCA, the electronic band structure with SOC along two magnetization directions [100] and [001] as well as MCA contribution at various k-points are analyzed for FeNi:N in Fig. 3. As the MCA depends on the electronic structure in the vicinity of EF (SOC constant of 3d TMs is very low $\sim$ 50-100 meV), the band structures are plotted only near EF. On analyzing band structures, it is found that difference in energies for both FeNi:N compounds is overall positive i.e. uniaxial anisotropy.

C-doped L10-FeNi:

Fig. 4(a) shows the schematics of the 221 supercell of base material FeNi which is needed to accommodate FeNi:C (Fig. 4(b)).

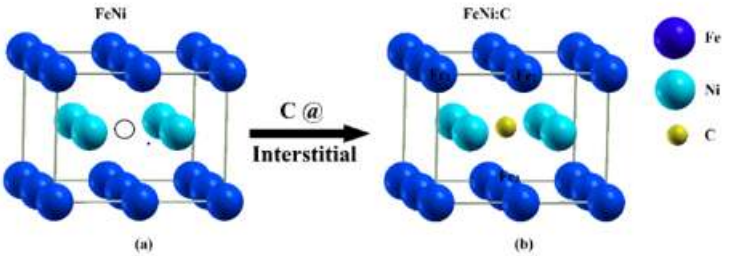


Fig. 4. Schematics of the 2×2×1 supercell of FeNi without and with interstitial C-doping: (a) FeNi (b) FeNi:C

TABLE 3. Optimized lattice parameters (in Å) and formation energy (E_{For}/f.u.) (in eV) of pristine and FeNi:C compounds

Compound	Lattice Parameters		c/a	E_{For}/f.u.
	a	c		
FeNi	2.531	3.579	1.414	-0.18
FeNi:C	2.541	3.799	1.495	-0.29

For investigation of electronic properties, total and orbital projected density of states (DOS) of FeNi and FeNi:C are depicted in Fig. 5. Total DOS of FeNi is spin polarized while on addition of C, some states are accommodated near the Fermi level (EF) in majority spin channel of FeNi:C which reduces its spin polarization. The new states at EF are appearing because of hybridization of Fe-3d and Ni-3d states with C-p states.

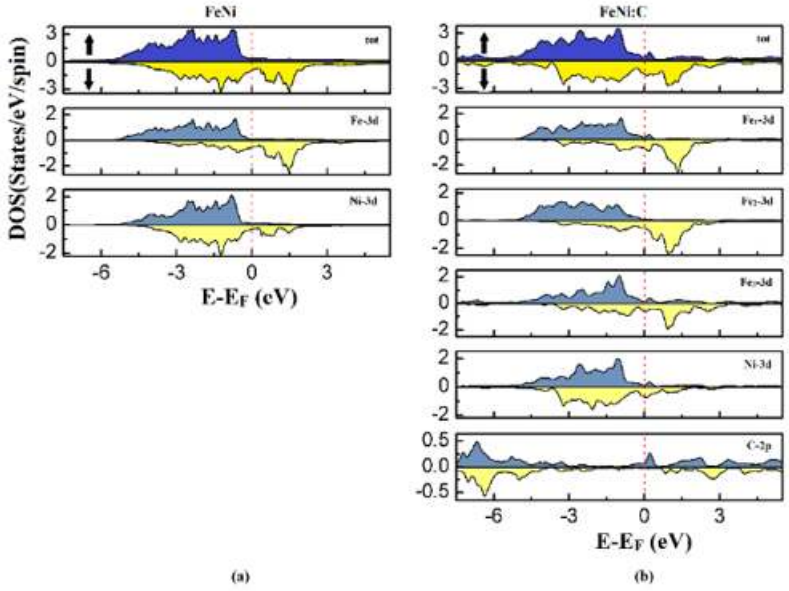


Fig. 5. Calculated total and orbital resolved DOS of (a) FeNi and (b) FeNi:C compounds

In FeNi:C, due to asymmetry caused by interstitial C-impurity, all Fe atoms can be categorized as three non-equivalent atoms as mentioned in Fig.5 by Fe1, Fe2 and Fe3. Now, total spin magnetic moment of FeNi:C decreases due to the hybridization of Fe3-3d/Ni-3d with non-magnetic impurity atom, C-2p. The calculated spin magnetic moments are isotropic for both the compounds. However, orbital magnetic moments are directional dependent and orbital moment anisotropy (OMA) defined by $\Delta\mu_{orb}=\mu_{orb}^{([001])}-\mu_{orb}^{([100])}$ is found as 0.005 B for Fe and -0.002 B for Ni in pristine FeNi and are in good agreement with Miuara et al. [19] The value of OMA increases to $\Delta\mu_{orb}(\text{Fe})=0.016\mu_B$ and $\Delta\mu_{orb}(\text{Ni})=-0.0003\ \mu_B$ on interstitial C-doping which is favorable to yield the increment in MCA.

TABLE 4. Calculated total and atom resolved spin magnetic moments, orbital magnetic moments, magnetization (M_S) and MCA (K) in of FeNi and FeNi:C compounds.

Compound	Direction	Magnetic Moments (μ_B)						M_S (T)	K (MJ/m³)
			Fe		Ni		Total		
FeNi	001	μ_s	2.701		0.645		3.271	1.32	0.43
		μ_l	0.054		0.036		-		
	100	μ_s	2.702		0.645		3.271		
		μ_l	0.049		0.038		-		
	Expt.	μ_s	2.540[16]		0.730[16]			1.47[14]	0.58-1.3[13-15]
		μ_l	0.050[17]		0.100[17]				
			Fe_1	Fe_2	Fe_3	Ni	C	Total	
FeNi:C	001	μ_s	2.610	2.906	1.802	0.486	-	2.996	1.13	1.88
		μ_l	0.056	0.057	0.041	0.024	0.038	-	
							0.001		
	100	μ_s	2.610	2.906	1.802	0.486	-	2.996	
		μ_l	0.050	0.046	0.010	0.023	0.038	-	
							0.001		

The calculated saturation magnetization (Ms) i.e. total spin magnetic moment per unit volume and MCA listed in Table 4. On C-doping, Ms decreases from 1.32 T to 1.13 T due to decrease in total spin magnetic moment. The calculated MCA of L10-FeNi is 0.43 MJ/m3 that is comparable with 0.47 MJ/m3 as calculated by Werwinski et al [18]. However, its experimentally measured value varies around 1 MJ/m3 [4-6]. On addition of interstitial C-doping, MCA increases to 1.88 MJ/m3. This increase can be attributed to the tetragonal distortion i.e. increased c/a ratio as examined by Miuara et al [19]. This increase can further be explained in terms of SOC between the states below and above the EF and importantly, this increase is inversely proportional to energy difference between occupied and unoccupied k states. In the vicinity of EF (Fig. 5), Eocc-Eunocc is smaller, FeNi:C contributes more states as compared to pristine FeNi that results in enhancement of MCA. Moreover, C-doping increases the anisotropy of the orbital moments in a direction i.e. favorable for MCA.

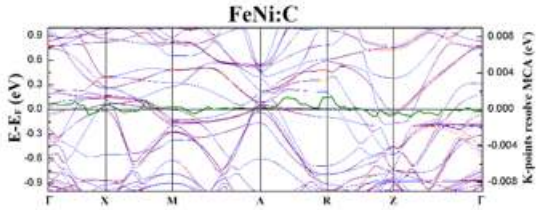


Fig. 6. Band structure including SOC with magnetization along [100] (black solid lines) and [001] directions (black dotted lines) along with the MCA contribution per k point (green) for FeNi:C.

In order to see the origin of the MCA, the electronic band structure with SOC along two magnetization directions [100] and [001] as well as MCA contribution at various k-points using the magnetic force theorem are analyzed for FeNi:C in Fig. 6. The band structures are plotted only in the vicinity of EF as the SOC constant of transition metals (TMs) is very low ∼ 50-100 meV. On analyzing band structures, it is found that difference in energies of FeNi:C along [100] and [001] directions is overall positive showing uniaxial anisotropy.

Cs-doped CH3NH3PbI3

Hybrid halide perovskites (HHPs) have emerged as a very promising candidate for absorber layer in third generation solar cells. Over the course of past few years, HHPs have taken the solar cell technology by storm as the solar cells based on these materials have exceeded

the photon conversion efficiency (PCE) to 23.3% [21] till date from 3.8% [22] in 2009. Such exponential rise in the PCE has never been witnessed before in any other existing solar cell technology. The factors that make HHP solar cells advantageous are their easy fabrication from the liquid phases [23] and the efficiency which can be tuned by controlling their structural order and composition [24].

HHPs have standard AMX3 perovskite structure, where X is the halide anion (Cl-, Br-, I-), M is the metal cation (Ge, Sn, Pb), while the remaining position A is taken by an organic molecule, generally methylammonium, CH3NH3 (MA) and formamidinium, HC(NH2)2 (FA) etc. MAPbI3 has been extensively applied owing to its ideal properties such as direct bandgap of 1.55 eV [25], high level of defect self-regulation [26], small exciton binding energy [27], excellent charge carrier mobility [28] and long charge carrier diffusion length [29]. But MAPbI3 based solar cells have failed to be commercialized due to lack of its intrinsic long term stability [30] and compositional degradation. Although ample efforts have been put by scientific community, both experimentally and theoretically in MAPbI3 yet addressing its long-term stability has always been a hurdle. So there is an imperative need to look for new HHP materials that are stable and efficient in ambient environmental conditions. It is established that the properties of the materials are closely related to their electronic structures so an intuitive strategy to achieve stability in the HHP absorber layer is to replace the cation A by suitable doping without compromising the excellent photovoltaic properties. Considering that, the structure of the HHP materials can be modulated by partial or full substitution of cation A with suitable cations like FA+ and Cs+ without destroying the Pb-I octahedral arrangement.

A lot of experimental efforts have been put in understanding physical properties of Cs-doped MAPbI3 but the theoretical investigations are rather limited. So the first principles calculations were carried out using DFT formalism as implemented in the VASP code [10] to systematically examine the geometry, electronic structure and optical properties of Cs-doped tetragonal MAPbI3 perovskite, which can be an alternative light absorber to MAPbI3. Furthermore, the relationship between structural, electronic and optical properties of pure and doped MAPbI3 have also been investigated. MAPbI3 adopts a tetragonal structure with space group I4/mcm at room temperature [31]. Interestingly, a tetragonal unit cell of MAPbI3 consists of 4 units of MAPbI3 with each Pb atom coordinates with six I-atoms (four in equatorial and two in apical direction). It has been confirmed experimentally that at the room temperature, the dipolar organic MA+ cation reorients quite rapidly [0.5-14 ps] inside the PbI6-octahedron cage [32].

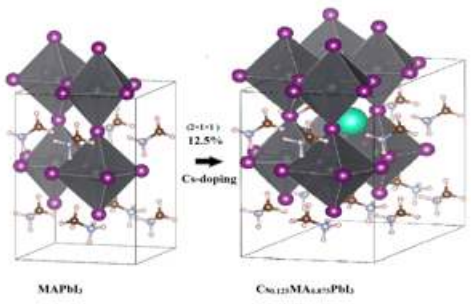


Fig. 7. Schematics for introducing 12.5% of Cs-doping in $MAPbI_3$ along with relaxed structures of $MAPbI_3$ and Cs:$MAPbI_3$. (Grey/Purple/Brown/Blue/Pink/Turquoise sphere represents Pb/I/C/N/H/Cs atom)

However, for computation, the MA+ cations have to be relaxed to fix orientations in such a way that there is minimum steric hindrance in the hybrid halide perovskite system. We used experi-

mental lattice parameters [33] as the input parameters of our DFT calculations and subsequently obtained the optimized local structure of MAPbI3 by applying the structural relaxation. In order to obtain 12.5% of Cs doping, a 211 supercell containing 8 formula units of MAPbI3 was formed and one MA+ ion was replaced by Cs+ within the supercell (Fig. 7). The optimized lattice parameters of pure and Cs:MAPbI3 obtained after relaxation are listed in the Table 5 which are in good agreement with experimental values [33] and other theoretical data [34].

TABLE 5. Calculated lattice parameters of $MAPbI_3$ and Cs:$MAPbI_3$

	$MAPbI_3$		Cs:$MAPbI_3$	
	a = b (in Å)	c (in Å)	a = b (in Å)	c (in Å)
This work	8.90	13.16	8.91	13.16
Experiment [33]	8.85	12.64	-	-
Theory [35]	8.89	12.70	-	-

The deviation in volume with respect to experimental data is less than 5% in case of MAPbI3. The incorporation of Cs in MAPbI3 doesnt have remarkable impact on the lattice parameters. But the hydrogen bonding existing between the H-atoms of MA+ cation and Iodine framework get reduced significantly which in turn increases the tilting of PbI6-octahedra. On measurement, we found that the minimum bond lengths of H-bond in Cs:MAPbI3 is 2.651 *AA* which is greater than that in MAPbI3 (2.627 *AA*), indicating that the strength of H-bonding gets reduced in doped lattice. Further, the average equatorial Pb-I-Pb angle gets increased from 152.10 to 153.97 on 12.5% of Cs-doping in MAPbI3. Therefore, the increase in tilt w.r.t. host MAPbI3 is 1.87 . On the other hand, the minimum bond length Pb-I covalent bonds decreases from 3.207 *AA* to 3.175 *AA* on this doping which yields the better strength of Pb-I bonds and the stability of Cs:MAPbI3 gets enhanced over pure MAPbI3. In this way, compositional degradation of MAPbI3 can be prevented and the solar cells based on it can be used for the longer time.

To explore the electronic structures of MAPbI3 and to see how Cs+ cation mixing affects the electronic properties of MAPbI3, the analysis of total density of states (DOS) was performed for both compounds. 12.5% of Cs doping drastically modifies the DOS in the energy region, -6.5 eV to -8 eV. Importantly, the DOS in sub - valence band maximum (VBM) region that is of interest for photovoltaic applications and as a result of cation mixing this DOS get enhanced in the region up to 0.5 eV below the VBM as evident from inset of Fig 8.

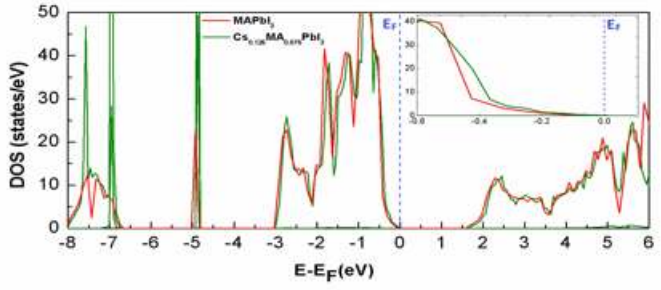


Fig. 8. Calculated TDOS of $MAPbI_3$ and Cs:$MAPbI_3$ at GGA level of theory

The magnitude of band gap of absorber material is very crucial as it is related to the maximum voltage of the PV device and determines the optical absorption [34]. The fundamental band gap (Eg) between the VBM and conduction band minimum (CBM) for MAPbI3 is 1.58 eV, which is in good agreement with the experimental value of 1.55 eV [25] as compared to previous

theoretical work [35] where value of Eg = 1.63 eV was reported.

To explain the above observations and to understand the bonding mechanism between the atoms of the Cs:MAPbI3, the analysis of partial density of states (PDOS) was performed. From panel 2, 3 and 4 of Fig. 8, it can be elucidated that the VBM is constituted of combination of Pb-6s and I-5p states.

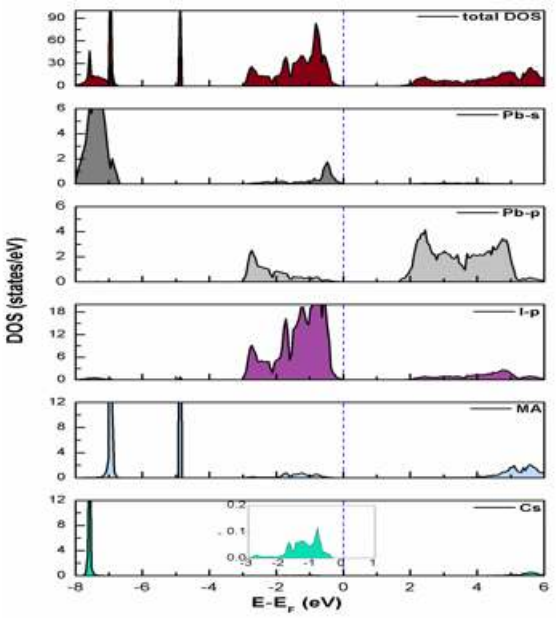


Fig. 9. Calculated Partial DOS (PDOS) of Cs:MAPbI$_3$ at GGA level of theory

Further, the inset of panel 6 of this figure also indicates a small contribution from Cs atom in the vicinity of EF which leads to a small shift of 0.04 eV in the band gap of the doped case w.r.t. host MAPBI3. The noticeable contribution of Cs is observed at $\sim$ -7.5 eV in the occupied region. Therefore, addition of Cs in MAPBI3 brings only the modest change in the band gap and optical response. On the other hand, the CBM is formed by the empty Pb-6p states along with a residual contribution from I-5p states. The first quantitative contribution ascribed to the MA+ cation is 5 eV deep in valence. The incorporation of Cs against CH3NH3 decreases the number of H-atoms and hence the overall strength of H-bonds between H and I gets reduced to some extent. Thus, in turn, increases the tilting of PbI6-octahedra and the coupling between Pb-6s and I-5p states becomes stronger which subsequently increases the band gap of resultant compound slightly.

The Fig. 10 shows the electronic charge density isosurfaces in the upper valence band and the lower conduction band. The delocalization of electronic charge on Cs-atom is clearly visible here.

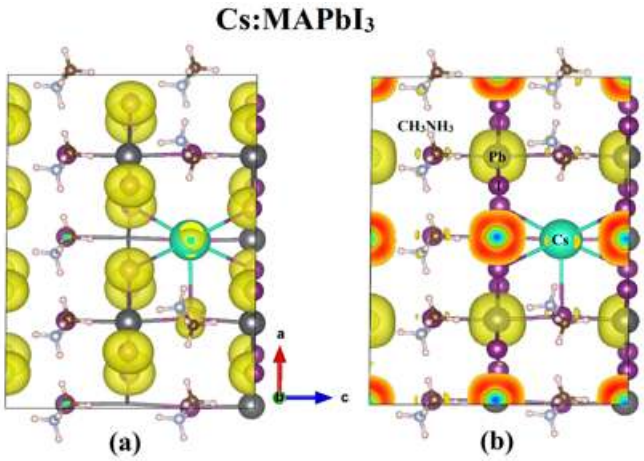


Fig. 10. Charge density isosurfaces of (a) the upper valence band and (b) the lower conduction band of Cs:$MAPbI_3$.

The electronic band structure of Cs:MAPbI3 along high symmetry points of the Brillouin zone is reported in the Fig. 11. The direct bandgap of 1.62 eV is obtained along the - direction. It is stressed here that the direct bandgap from the dispersed Pb-6s/ I-5p valence bands to Pb-6p conduction bands plays an essential role in the superior PV performance of the PSCs and all the visible light absorption takes place in the inorganic cage structure with almost no light absorption by central cation.

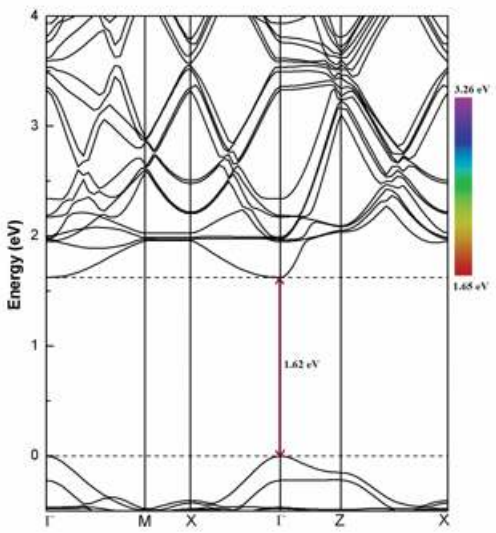


Fig. 11. Bandstructure of Cs:$MAPbI_3$ along some high symmetry points of the Brillioun zone

The optical absorption between of these materials is closely related to their electronic structures. The edge transition in both the compounds comes from mixed Pb-6s, I-5p to Pb-5p states. The intra-atomic transition probability is high which accounts for the higher value of absorption coefficient in both as compared to other commonly used PV materials [35]. Moreover, the value of absorption coefficient in Cs:MAPbI3 is higher than that of MAPbI3 in the visible energy range i.e. from 1.62 eV to 3.25 eV [36] making it one of the potential candidates for the absorber layer in PSCs (Fig. 12). The optical absorption is decided by the trade-off between widening of the band gap and increase of DOS in sub-VBM region at a particular doping concentration. For 12.5% of Cs doping in MAPbI3, increased DOS in the sub-VBM accounts for the increased absorption coefficient.

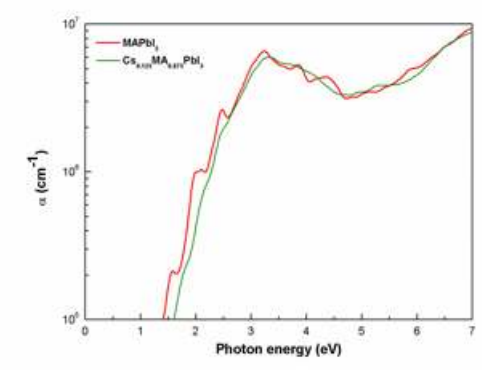


Fig. 12. Absorption coefficient of $MAPbI_3$ and Cs:$MAPbI_3$

Hence, Cs-doing offers an alternative way to avoid the compositional degradation of MAPbI3 at no cost of optical absorption and the photovoltaic performance of MAPbI3 based solar cell device can be extended for a longer time.

Cs2+ doped HC(NH2)2PbI3 (FAPbI3)

FAPbI3 adopts a cubic structure with space group Pm-3m at room temperature. In a unit cell of FAPbI3 each Pb atom coordinates with six I-atoms (four in equatorial and two in apical direction. For computation, the FA+ cation has been relaxed to a fixed orientation. We used experimental lattice parameters as the input parameters of our DFT calculations to obtained the optimized local structure of FAPbI3.

In order to obtain 12.5% of Cs doping, a 222 supercell was formed and one FA+ ion was replaced by Cs+ within the supercell (Fig. 13). Doping concentration beyond 12.5% has been avoided as increased Cs content would have undesirably enhanced the bandgap value.

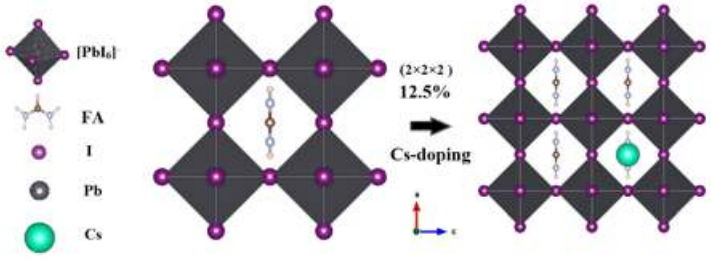


Fig. 13. Schematics for introducing 12.5% of Cs-doping in $FAPbI_3$

The incorporation of smaller Cs in FAPbI3 reduces the lattice parameters and hence cubo-octahedral volume which leads to stronger interaction between FA+ and iodine framework. This enhanced interaction imparts stability to the Cs:FAPbI3 HHP.

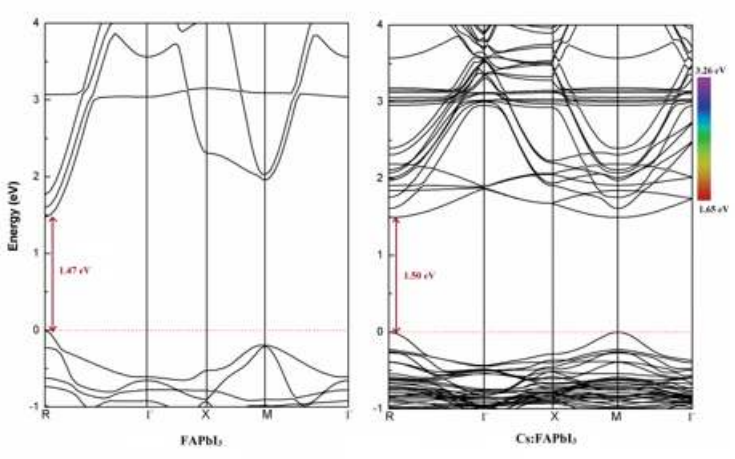


Fig. 14. Bandstructure of $FAPbI_3$ and $Cs:FAPbI_3$ along some high symmetry points of the Brillioun zone

The electronic band structure of FAPbI3 and Cs:FAPbI3 along high symmetry points of the Brillioun zone is reported in Fig. 12. The fundamental bandgap (Eg) of 1.47 eV is obtained between valence band maxima (VBM) and conduction band minima (CBM) along the R- R direction in FAPbI3 which is in good agreement with experimental value of 1.48 eV [37]. However, this agreement is due to counterbalance of GGA underestimation by overestimation of values due to the lack of spin-orbit interaction. Post Cs doping, a slight blue shift is observed and the value of Eg got increased to 1.50 eV, which signifies that material has retained the photovoltaic properties at 12.5% of Cs doping. The blue shift is due to decreased lattice constant on Cs doping.

Similar to the MAPbI3, in FAPbI3 the band edges are contributed mainly from PbI6 octahedra whereas the contribution of FA+ lies deep inside the valence band. The edge transition in both the compounds comes from mixed Pb-6s, I-5p to Pb-5p states.

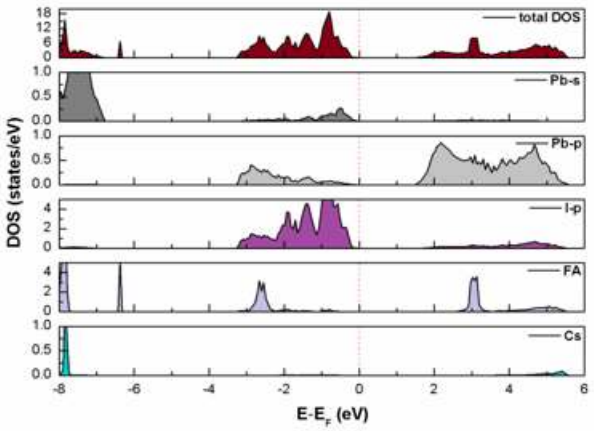


Fig. 15. Calculated Partial DOS (PDOS) of $Cs:FAPbI_3$ at GGA level of theory

The intra-atomic transition probability is high which accounts for the higher value of absorption coefficient in both as compared to other commonly used PV materials. The value of absorption coefficient in Cs:FAPbI3 is higher than that of FAPbI3.

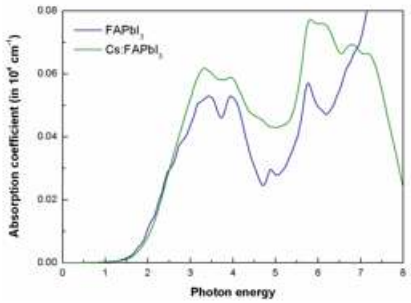


Fig. 16. Absorption coefficient of $FAPbI_3$ and $Cs:FAPbI_3$

Our results show that decreased cubo-octahedral volume post Cs-doping not only impart the stability to FAPbI3 but also increases the bandgap to 1.50 eV. Furthermore, an enhanced value of absorption coefficient was observed in the visible light region for the Cs:FAPbI3.

Publications / Articles etc. (If any):

1. Magnetocrystalline anisotropy of Pt-doped L10-FeNi compound for clean energy applications, Priti Rani, Jyoti Thakur, Ankur Taya and Manish K. Kashyap, , Vacuum 159, 186 (2019).

2. Ankur Taya, Priti Rani, Jyoti Thakur and Manish K. Kashyap, First principles study of structural, electronic and optical properties of Cs-doped CH3NH3PbI3 for photovoltaic applications, Vacuum 160, 440 (2019).

3. Effect of tetragonal distortion induced by interstitial C-doping in L10-FeNi, Priti Rani, Jyoti Thakur, Ankur Taya and Manish K. Kashyap, Accepted in AIP Conference Proceedings (DAE SSPS 2018).

4. Ankur Taya, Priti Rani and Manish K. Kashyap, First Principles study of structural, electronic and optical properties of Pb-based Hybrid Halide Perovskites , Accepted in AIP Conference Proceedings (DAE SSPS 2018).

5. Ankur Taya, Priti Rani and Manish K. Kashyap, Structural, Electronic and Optical studies of Pb-Free Halide Double Perovskite Cs2BiAgBr6; an mBJLDA approach, Accepted for AIP Conference Proceedings (RACMP-2018).

Awards (If any):

Best poster award on Enhanced optical properties via cation doping in Hybrid Lead Iodine Perovskites to Ankur Taya, Priti Rani and Manish K. Kashyap in International workshop on Evolution of Electronic Structure Theory & Experimental Realization (EESTER-2018) organized by SRM-IST and IIT Madras from September 11, 2018 to September 15, 2018.

Work presented in conference/s with photographs (if any):

1. A paper entitled Analyzing magnetic anisotropy of Pt-doped L10-FeNi compound for permanent magnets presented in 6th National Conference on Nanoscience and Instrumentation Technology organized by Department of Physics, NIT Kurukshetra-136119, Haryana during March 29-30, 2018.

2. A paper entitled Magnetocrystalline anisotropy of Pt-doped L10-FeNi compound for clean energy applications presented in International Symposium on Functional Materials (ISFM-2018) organized by IIT Kanpur, Punjab University Chandigarh and University of Illinois at Chicago during April 13-15, 2018.

3. A paper entitled First principles investigation of electronic properties and magnetic response of Fe3Co3Ti2 in non-cubic phase presented in Two Day National Conference on Recent Advances in Condensed Matter Physics organized by Department of Physics, Kurukshetra University, Kurukshetra, Haryana during October 12-13, 2018.

4. A paper entitled Effect of tetragonal distortion of L10-FeNi by C/N interstitial presented in International workshop on Evolution of Electronics Structure Theory & Experimental Realization (EESTER-2018) organized by SRMIST & IITM, Chennai during September 11-15, 2018.

5. A paper entitled Effect of tetragonal distortion on magnetocrystalline anisotropy and magnetism of L10-FeNi:N presented in International Conference on Magnetic Materials and Applications (ICMAGMA-2018), is being jointly organized by NISER, Bhubaneswar and MSI during 9-13 December, 2018.

6. A paper entitled Effect of tetragonal distortion induced by interstitial C-doping in L10-FeNi presented in 63rd DAE SSPS held in GJU S&T, Hisar, Haryana during 18-22 December, 2018.

7. A paper entitled Effect of Cs2+ doping on structural, electronic and optical properties of Methyl ammonia lead iodide presented by Ankur Taya and Manish K. Kashyap in 6th National Conference on Nanoscience and Instrumentation Technology (NCNIT-2018) at National Institute of Technology, Kurukshetra during March 29-30, 2018.

8. A paper entitled First Principles study of Structural, electronic and optical studies of lead based hybrid halide perovskites presented by Ankur Taya, Priti Rani and Manish K. Kashyap in International symposium on Functional Materials (ISFM-2018): Energy and Biomedical applications at Hotel Shivalikview, Chandigarh jointly organized by IIT Kanpur, UIC-USA and Chandigarh University during April 13-15, 2018.

9. A paper entitled First Principles study of structural, electronic and optical properties of Lead-based Hybrid Halide Perovskites presented by Ankur Taya, Priti Rani and Manish K. Kashyap in International Workshop on Evolution of Electronic Structure Theory & Experimental Realization (EESTER-2018) organized by SRM Institute of Science and Technology & Indian Institute of Technology Madras in association with MRSI computational materials science subject group at Chennai during September 11-15, 2018.

10. A paper entitled First Principles study of structural, electronic and optical properties of Cs- doped HC(NH2)2PbI3 for photovoltaic presented by Ankur Taya, Renu Singla, Priti Rani, Jyoti Thakur and Manish K. Kashyap in 63rd DAE Solid State Physics Symposium (DAE-SSPS 2018) at Guru Jambheshwar University of Science and Technology (GJUS&T), Hisar, Haryana during December 18-22, 2018.

Appreciation / Recognition (if any):N/A

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Benefits & experience of using NPSF:

The work involved under our project requires heavy computational resources. On ordinary machines or servers, this type of work cant be possible. We are fortunate to have C-DACs NPS facility which enabled us to perform complex computational work involving Density Functional Theory (DFT) calculations. We have sometimes utilized more than 100 cores to perform the calculations of hybrid halide perovskite materials and these calculations were completely in efficient time frame always. Without NPSF facility, the theoretical research involving heavy computation can never to thought. The queuing system to fire the job is wonderful, it gives the equal chance for every user to submit their job. The NPSF staff members are very helpful and cordial. They helped us time to time in writing the script and installation of some software in our account. We are thankful to supporting staff of NPSF for making all the computational work possible for us.

Any other relevant information (if any): No

Title of the work carried out: Sensing Properties of magnetic cluster

Name & Designation of the Chief Investigator: Dr. Mrs. M. D. Deshpande, Designation : Professor

E-mail Id: d_mrinal@yahoo.com

Institution Name: H. P. T. Arts & R. Y. K. science, College, Nasik

Research Challenge/s:

To calculate structural, electronic, magnetic and optical properties of clusters. It is challenging to calculate magnetic and optical properties of clusters. The study will be use as a basis for experimental activity for the development of nanosensors.

Work carried , Milestone, Achievements & Graphs, Plots:

We are working on superparamagnetic Iron oxide nanoclusters .

Publications / Articles etc. (If any):

Work is in progress.

Awards (If any): -

Work presented in conference/s with photographs (if any) -

Appreciation / Recognition (if any): -

Benefits & experience of using NPSF:

NPSF technology provide easy access and helped us for scientific application to carry out our research work.

Any other relevant information (if any):

Title of the work carried out: Ab initio Molecular Dynamics Simulations, Electronic Structure, Magnetic and Spectroscopic Properties of Nano materials and Bimolecular Interfaces

Name & Designation of the Chief Investigator: Dr. Md. Ehesan Ali, Scientist-E

E-mail Id: ehesan.ali@inst.ac.in

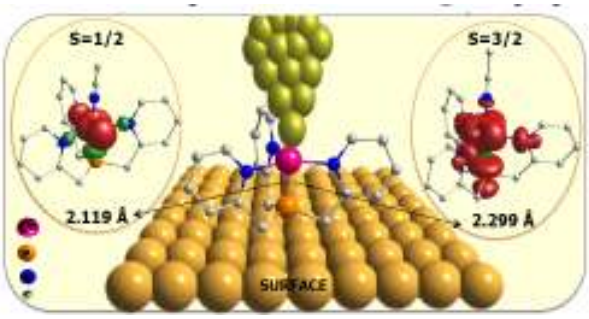
Institution Name: Institute of Nano Sciences and Technology

Research Challenge/s:

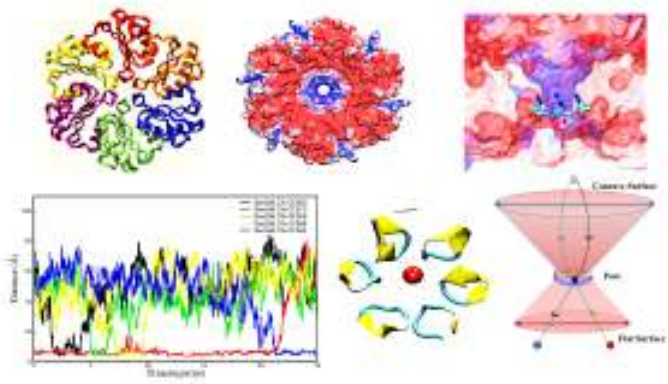
1. Understanding the electron and spin-injections across the Biomolecule-Nanomaterials interface
2. Designing of stable organic diradicals with tunable and ferromagnetic magnetic exchange interactions
3. Spin-crossover properties in Single-molecule Magnets

Work carried, Milestone, Achievements & Graphs, Plots:

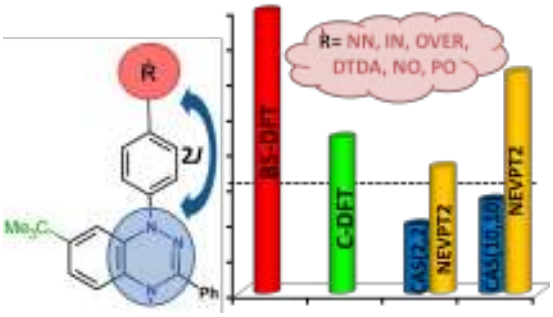
1. We have designed Co(II)-complex based single molecule magnet (SMM) that exhibits chemical-bond induced spin-crossover properties.



2. We have captured the Ion-transfer dynamics for BMC protein



3. Blatters diradical and its observed exchange interactions are investigated in various state-of-the-art computational techniques and predicted various similar diradicals with strong Exchange Interactions.



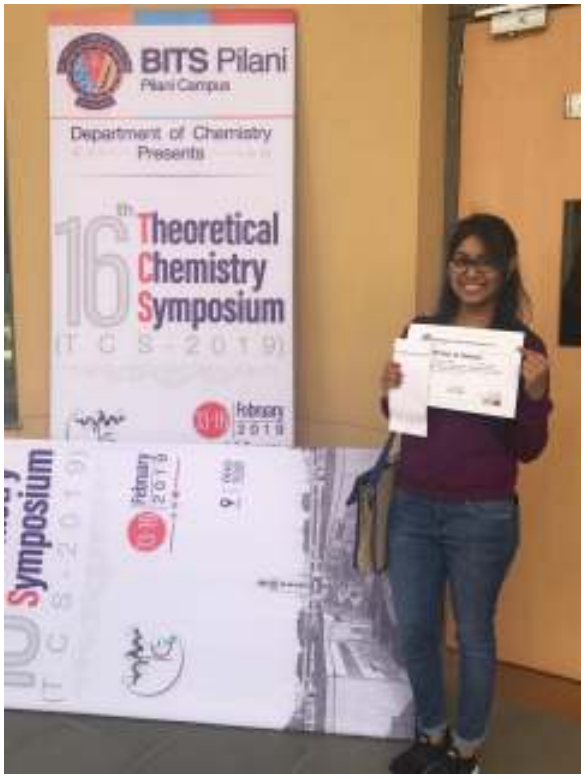
Publications / Articles etc. (If any):

1. Rai, R. et al. Environmentally Benign Metal-Free Reduction of GO Using Molecular Hydrogen: A Mechanistic Insight. ACS Omega 3, 1511215118 (2018).

2. Kathewad, N., Pal, S., Kumawat, R. L., Ehesan Ali, M. Khan, S. Synthetic Diversity and Luminescence Properties of ArN(PPh 2) 2-Based Copper(I) Complexes. Eur. J. Inorg. Chem. 2018, 2518-2523 (2018).

Awards (If any):

Ms. Prabhleen Kaur received best poster presentation in Indo-French Conference on Molecular Magnetism held at IISc Bangalore November 26-30, 2018



Ms. Ashima Bajaj Received the best poster prize in Theoretical Chemistry Symposium held at BITS-Pilani, February 13-16 2019.

Work presented in conference/s with photographs (if any)

1. Theoretical Chemistry Symposium, BITS Pilani, November 13-16, 2019
2. International Conference on Vector Born Diseases, Bhubaneswar, January, 9-11, 2019
3. International Conference on Magnetic Materials and Applications (ICMAGMA-2018), Bhubaneswar, December 9-13, NISER Bhubaneswar
4. Indo-French Conference on Molecular Magnetism, IISc Bangalore November 26-30, 2018

Appreciation / Recognition (if any):

References:

Benefits experience of using NPSF:

The computing resources provided by NPSF is indeed a great help to us as it mostly fulfils our growing needs of the computing resources to pursue world class research activity without developing any local HPC. This is indeed a great initiative by Govt. of India to provide resource to the researcher of relatively smaller institute that the lack of appropriate man power to manage a data center and generate such huge scale of computing resources. I must appreciate help from NPSF experts and various supporting staffs. They are always easy to approach and quick to resolve the issues related to all issues.

Any other relevant information (if any):

Title of the work carried out:gas sensing properties of graphene based materials : Density Functional Theory

Name & Designation of the Chief Investigator: Dr. Mrs. M. D. Deshpande, Designation : Professor

E-mail Id: manasi.mahabal@gmail.com

Institution Name: H. P. T. Arts & R. Y. K. science, College, Nasik

Research Challenge/s:

To calculate electronic, optical, and transport properties at the atomic scale. It is challenging to calculate the transport properties for the device application.

Work carried , Milestone, Achievements & Graphs, Plots:

The understanding of structural, electronic, magnetic and optical properties of functionalization of nanosheets with metal for applications such as sensors, device fabrication. We are basically working on the gas sensing properties of the graphene based materials. Now based on earlier study, our interest is to study the BN functionalized graphene nanosheet with greenhouse as well as toxic gas molecules. These studies will be useful for the improvement of sensitivity of the graphene based gas sensor. It will provide strong base for experimentalist to carry further development in the sensor application,

Publications / Articles etc. (If any):

Rare earth dopant effects on optical properties of Alumina : DFT study IJCPS March 2018

Awards (If any):

Best oral presentation at ICAFM 2018, Nasik

Work presented in conference/s with photographs (if any) :

1. Oral presentation at International Conference on Advances in Functional Materials (ICAFM)- 2018 at K. T. H. M. College, Nasik
2. Poster presentation at Advanced Materials Synthesis, Characterization and Applications (AMSCA 2018) at Department of Physics, S. P. Pune University.

Appreciation / Recognition (if any):

References:

Benefits & experience of using NPSF:

The purpose of NPSF for the contribution of parallel and distribute processing technologies in India which in turn helped for us for the scientific applications to carry out research more effectively.

Any other relevant information (if any):

Title of the work carried out: Dimeric stability of the NS1 protein of ZIKA virus

Name & Designation of the Chief Investigator: Dr. Neelanjana Sengupta, Assistant Professor

E-mail Id: senguptan@gmail.com

Institution Name: Indian Institute of Science Education and Research Kolkata

Research Challenge/s:

Work carried , Milestone, Achievements & Graphs, Plots: See attached report

Publications / Articles etc. (If any): NA

Awards (If any): NA

Work presented in conference/s with photographs (if any): NA

Appreciation / Recognition (if any): NA

References: See attached report

Benefits & experience of using NPSF:

We are very much greatfull to the NPSF team for providing the computational resource in support of our project and the technical helps we got it is highly appreciated.

Any other relevant information (if any): NA

Introduction

Zika virus is a arbovirus belongs to the flavivirus family[1] and the epidemics of this virus in 2015 given rise to severe neurological complications[2]4 . The spread is mainly facilated by the mutation in NS1 which causes more antiganaemia[5]7 and inhibit the interferon beta-induction[8] . NS1 is a multifunctional non-structural protein[9] . This protein secreted from cell as hexamer which is a potential biomarker. Inside the cell, NS1 present as dimeric protein anchored to the membrane and forms replication complex[9,10] . Each of the NS1 monomer has three domains: beta hairpin (1 to 30 residues), wing (31 to 175 residues) and ladder (176 to 352 residues) 11 . The beta-ladder domain consists half of the monomers and provides stability as backbone 11,12 .

Methodology

System setup

To study the role of ladder domain in the dimer form, 176 to 352 residues of both the monomer were selected from the full NS1 dimeric protein (Protein Data Bank (PDB) entry 5GS6) 11 . The system created without any change considered as unperturbed system. Two restrained systems (Figure 2 (a)) were created to restrict the conformation by torsional restrain of spaghetti loop (219 to 273 residues) of monomer 1 and both the monomers respectively based on the PDB structure. Each of the ladder domain has four intra disulfide bonds (Figure 3 (a)). Four disulfide perturbed systems were generated by reducing disulfide bond one by one of each of the monomer respectively. In all the systems, protein was solvated with TIP3P 13 water model by keeping the protein $15AA$ away from the edge of resulting simulation box. All the system preparation and visualization is done with VMD 14 .

Simulation details

NAMD 2.12 15 simulation package with CHARMM22 force field with the CMAP corrections 16,17 used for the simulation. Simulation was done in three steps: minimization, equilibration followed by production run in NPT ensemble. The minimization was carried out in the conjugate gradient method for 40ps. The time step of 2fs was used. Periodic boundary conditions was orthorhombic and particle mesh Ewald (PME) 18 method applied in the long range electrostatics calculation. Non-bonded interactions were considered within the range of $12AA$. To maintain the constant temperature and presssure, the Langevin dynamics with a collision frequency of 1 ps 1 and the NosHoover Langevin piston 19 was used respectively. Hydrogen atoms mediated bonds constraints with the SHAKE algorithm 20 . After the minimization, heating was done at 310K for 1ns and followed by 20ns of equlibration. In the last step of production run, 250ns of trajectory generated which is used in the analysis.

Results and discussion

In first year we have reported that the system stabilty along the 30ns of simulation time. The backbobe RMSD (Root mean squared deviation) and Rg (Radius of gyration) shown the system was stable; Contact area (SASA of dimer - (SASA of Monomer 1 + SASA of Monomer 2), COM (Center of mass) distance between two monomers, interaction energy (kcal/mol) also shown the two monomers were not diffused out indicationg a strong intra and inter stability.

1. Dynamics of unperturbed system

The system is stable along the 0.5 microsecond of simulation time window which is proved by the backbone RMSD anaysis of the system (Figure1.(a)). In the MSF study two of the monomers fluctuating with similar intensity showing the homogeneity in the dimer. Interstingly the residues belongs to the spaghetti loop (SL) were fluctuating similar to the structured regions (Figure 1 (b)). The secondary structure analysis reveals evolution of a transiently new 3 10 helix in the SL region which supported the reduced fluctuation in the MSF analysis (Figure 1 (c)). In the inter contact area map, eight contact cluster emerged which stabilizing the internal stability between the monomers. The ranking of these clusters based on contact numbers. Among these clusters two highly ranked clusters i.e. C1 and C2 providing major support to the overall interaction. The C1 and C2 were predominantly hydrophobobic and polar and these clusters present in the outer and innner face of the ladder dimer respectively (Figure 1 (d)).

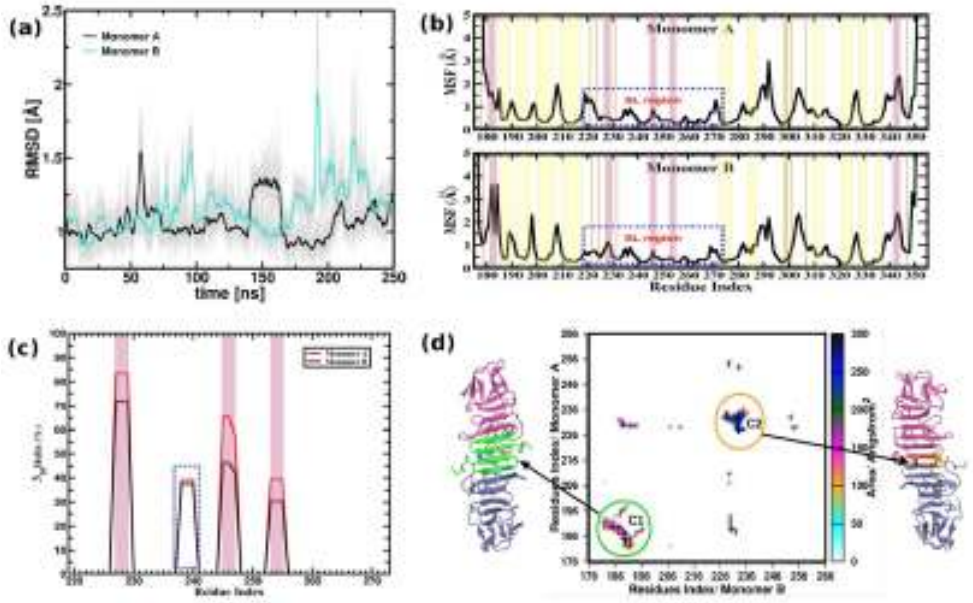


Figure 1. Dynamic stability of unperturbed ayatem. Root mean squared deviation (RMSD) along the time (a) and residue wise average mean squared deviation (MSF) (b) of ladder domain of two monomers. Residue-wise percentage of 3 10 helix content (c)of spaghetti loop and inter-contact map based on area.

2. Effects of conformational restraints

The C2 cluster present in the SL region and this region shown conformational switching. To understand the role of the SL into the dimeric stability we have imposed torsional restrained based on the experimental results to restric the structural changes. The interaction energy analysis suggests that the strong interaction between the ladder domain depends on the shuffling of conformations in the spaghetti loop (SL) region. The weakening of C2 much more than C1 supported that the ladder domain interaction mediated by conformational switching of spaghetti loop (Figure 2).

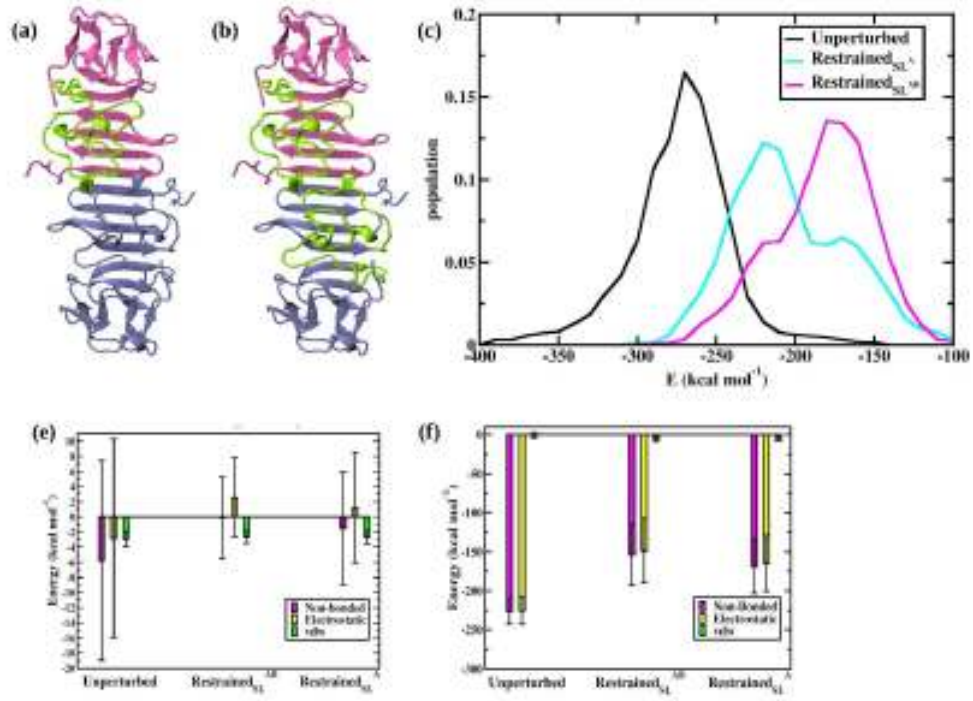


Figure 2. Effects of conformational restraints. The restrained spaghetti loop in Restarined SL A (a) and Restarined SL AB (b) shown in green. Probability distribution of total interaction energy (c), averaged interaction energy of C1 and C2 between two ladder domain of unperturbed, Restarined SL A and Restarined SL AB systems.

3. Effects of increased randomness by reducing disulfide bonds

Reduced conformation conversion weakens the interaction. In each of the ladder domain four disulfide bonds were present named as DS1, DS2, DS3 and DS4. Usually disulfide bond plays an important role in restricting the movement at the tertiary level of protein folding. One residue of DS1 bond was present in the spaghetti loop region which might be the constrain factor of randomness. To elevate the fluctuations and understand the role of each disulfide bond we have reduced it in both the domains. As expected, the backbone RMSD was increased for all the reduced system but DS3 and DS4 reduced systems shown comparatively lesser degrees of deviation than DS1 or DS2 purterbed systems. Interestingly, in the MSF analysis it was noticed that the heterogeneity of fluctuations in the homodimer due to DS1 perturbation.

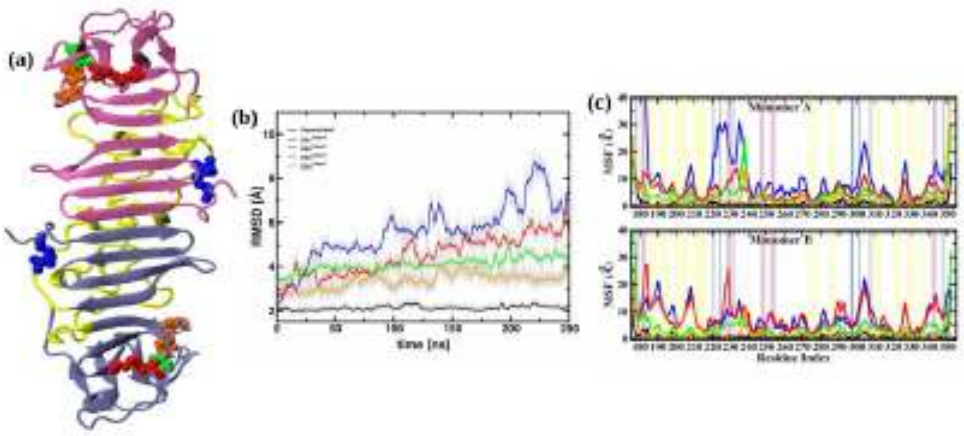


Figure 3. Effects of randomness due to reduction of disulfide bonds. Location of intra disulfide bonds on the ladder domain. Disulfide bond 1 (DS1), disulfide bond 2 (DS2), disulfide bond 3 (DS3) and disulfide bond 4 (DS4) were shown in blue, red, green and orange respectively (a). Backbone RMSD (b) and residue-wise mean sqared fluctuations (MSF) after reducing the same disulfide bond of ladder dimer

4. Increment of fluctuations altered the contacts in the perturbed systems

In the differential (purterbed - unperturbed) contact area map, most of the C1 contacts losses or weakens but in DS1 and DS2 reduced systems some transiently new contacts emmerged. C2 contacts also affected by these perturbations but in the DS3 and DS4 perturbed systems very few number of contacts lost or more or less same type of contacts like unperturbed system.

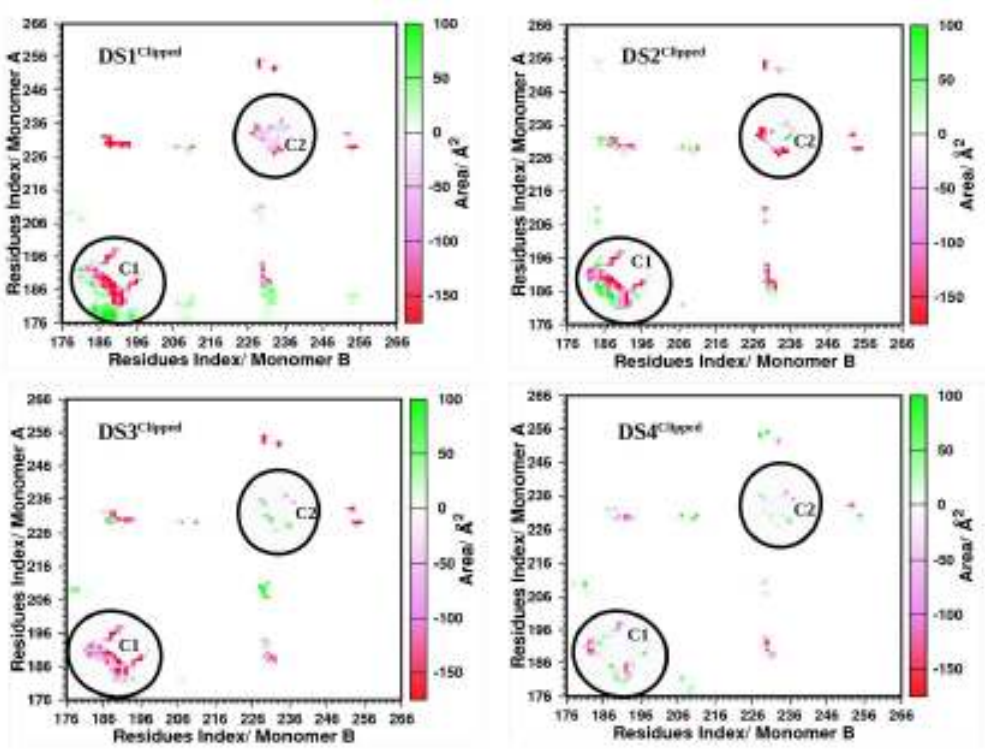


Figure 4. Differential inter contact map of perturbed systems. The encircled areas denotes cluster 1 (C1) and cluster 2 (C2) respectively.

5. Weakening of interactions

The loss of contacts in the DS1, DS2 and DS3 perturbed systems causes weakening of interaction between the monomers. The weakening due to DS1 was started after 200ns of simulation and C2 weakening was predominantly affected it. But the C1 interaction increases due to transient new contacts in the DS1 reduced system. Interestingly, DS2 perturbation which was 30A apart from both the C1 and C2 causes early weakening in a sequential manner and affects the both (i.e. C1 and C2) the cluster and DS4 perturbation was strengthens the interaction

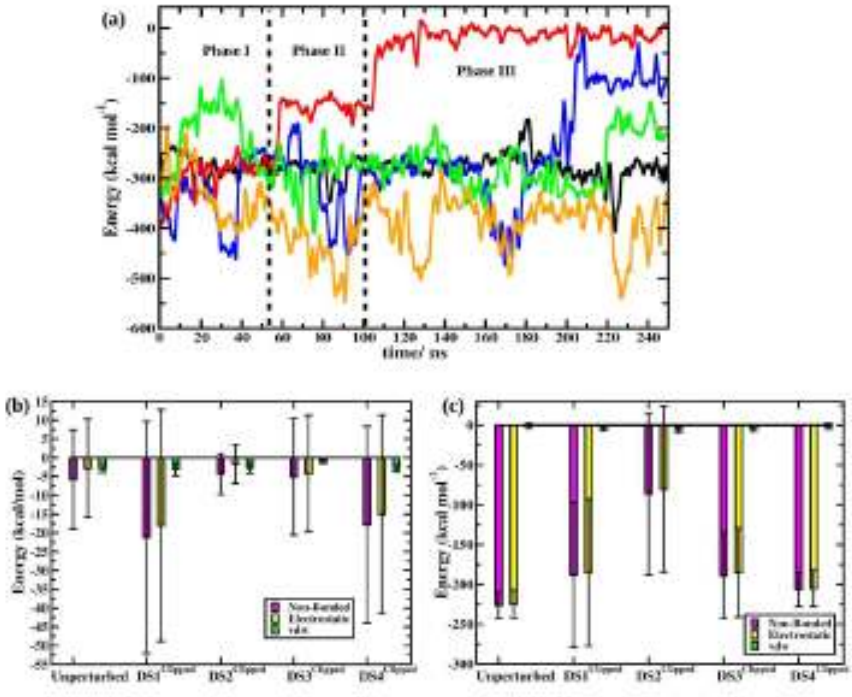


Figure 5. Total interaction energy between the two ladder domain along the time. Black, blue, red, green orange denotes Unperturbed, DS1 Clipped , DS2 Clipped , DS3 Clipped and DS4 Clipped systems respectively The area separeted by dotted line named as phase based on the DS2 perturbation mediated weakening (a). Averaged interaction energy of C1 (b) and C2 (c) between two ladder domains.

6. Mechanistics of DS2 reduction mediated weakening

The pair-wise interaction energy of C2 analysis shown that the weakening was due to breakage of two salt bridges. The H-bond of SB1 and SB2 weakens in the Phase II and Phase III respectively.

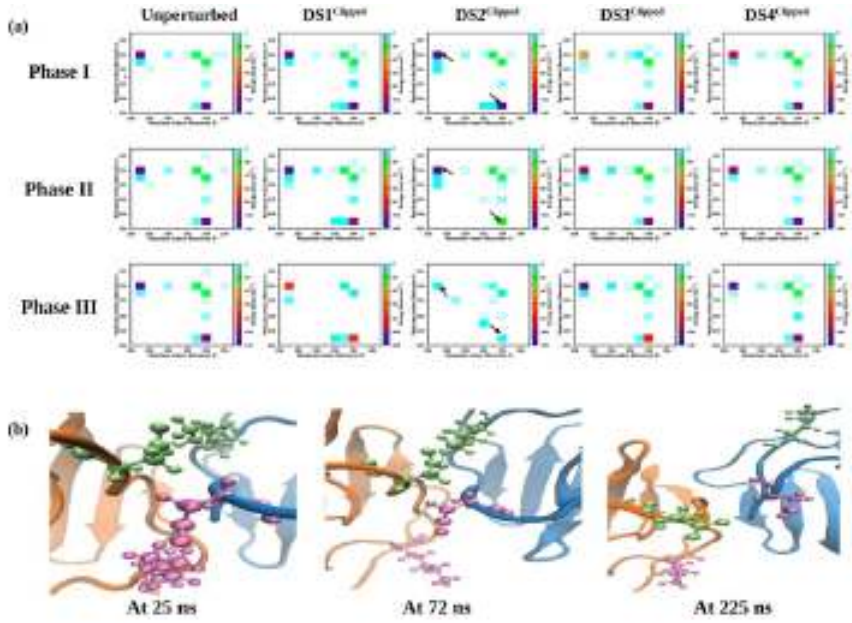


Figure 6. Contact energy map of C2 of unperturbed and perturbed systems. The arrow denotes

the sequential weakening of salt bridge (SB) 1 and 2 (a) and breakage of salt bridge at three different time comparable to the phases (b) in DS2 Clipped system.

7. Emergence of three new salt bridges in the DS4 reduced system

The strong interaction between the ladder domain in the DS4 reduced was not due to the C1 or C2. In the pair-wise energy contact map except the C1 and C2, three new salt bridges came out which mainly stabilize the interaction. The new salt-bidges presents nearby to C1 cluster. Figure 7. The residues which only formed salt bridges in the DS4Clipped system were shown (a). Residue-wise energy conatact map of 177 to 183 and 205 to 211 residues of DS4Clipped system (b). Distance distribution of SB3, SB4 and SB5 of unperturbed and disulfide perturbed systems (c).

Conclusion

The perturbations either by conformation restraints or increased randomness affects the interaction between the monomers. The DS1, DS2 and DS3 reduction causes structural changes, dynamic heterogeneity and loss of contacts which were crucial factors for dimeric stability. Interestingly, the DS4 reduction causes strong interaction which was different effect than other disulfide bonds. The DS1 reduction mediated weakening started at the end of our simulation time window. To validate our results we needs to do statistically significant amount of simulations.

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Title of the work carried out:

1. Performance of space-time coupled least-squares spectral element methods for parabolic problems
2. Space-time coupled least-squares spectral element methods for parabolic problems

Name & Designation of the Chief Investigator: Dr Pankaj Biswas, Assistant Professor.

E-mail Id: pankaj.biswas2002@gmail.com, pankaj@math.nits.ac.in

Institution Name: NIT Silchar, Assam, INDIA

Research Challenge/s:

We considered a one dimensional convection diffusion problem which possess a boundary layer at one end. Due to the presence of boundary layer conventional methods does not give satisfactory results. We consider geometric mesh near the boundary layer and perform spectral element method on parallel computers.

Work carried , Milestone, Achievements Graphs, Plots:

We have published two papers and presently working on One dimensional convection diffusion problem using spectral element method using parallel computers. For graphs we refer the published papers.

Publications / Articles etc. (If any):

1. Performance of space-time coupled least-squares spectral element methods for parabolic problems, P Biswas, NK Kumar, AK Kar, Journal of Physics: Conference Series 1132 (1), 012020
2. Space-time coupled least-squares spectral element methods for parabolic problems, P. Biswas, P. Dutt, S. Ghorai and N. Kiskore, Kumar, Accepted in International Journal for Computational Methods in Engineering Science Mechanics.

Awards (If any):

Work presented in conference/s with photographs (if any):

1. 3rdInternational Conference on Mathematical Sciences and Statistics(ICMSS2018), 6-8th Feb, 2018, Putrajaya, Malaysia, Performance of space-time coupled least-squares spectral element methods for parabolic problems, P Biswas, N K Kumar, A K Kar, Journal of Physics: Conference Series 1132 (1), 012020
2. ICM, Rio De Janerio, Brazil, 1 Aug 2018 9 Aug 2018, Performance of Spectral Method for Parabolic Problems, P Biswas

Appreciation / Recognition (if any):

References:

Kindly find the published papers.

Benefits & experience of using NPSF:

I have used NPSF super-computing facility for parallel computations.

Any other relevant information (if any):

Title of the work carried out: Noble metal nanostructures: nanotubes and nanoribbons

Name & Designation of the Chief Investigator: Prof. P. K. Ahluwalia

E-mail Id: pupooja16@gmail.com

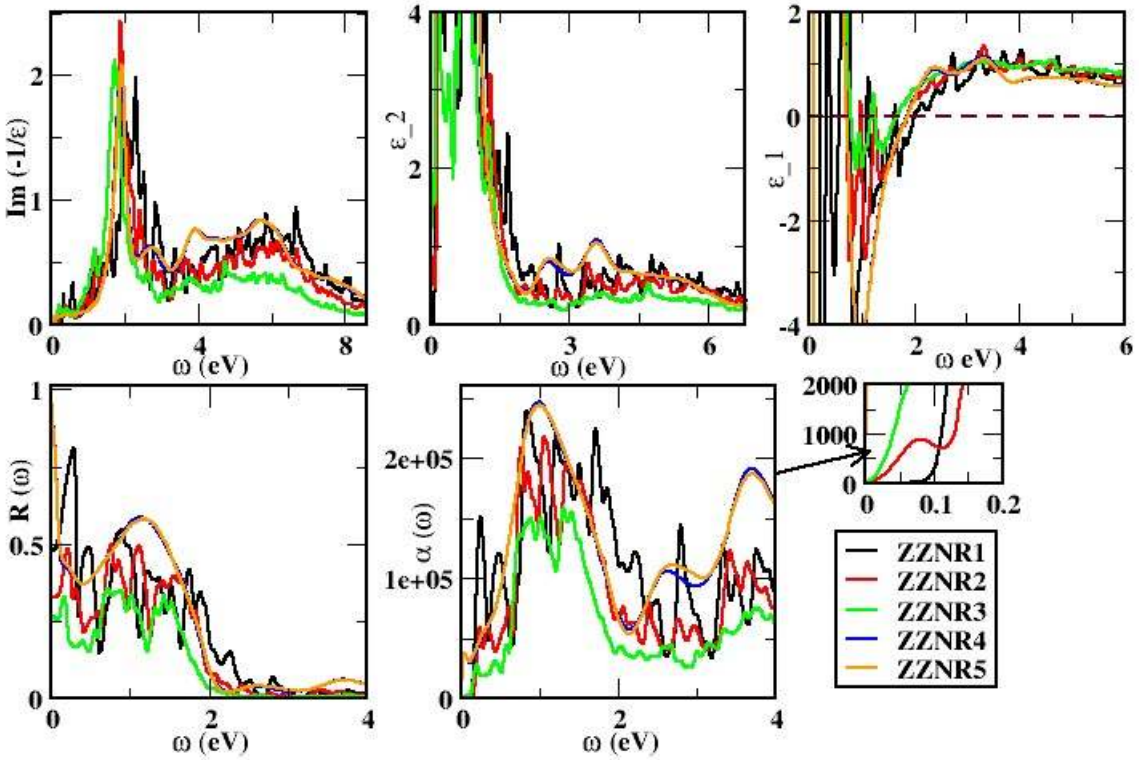
Institution Name: Physics Department, H. P. University, Shimla (H.P.)

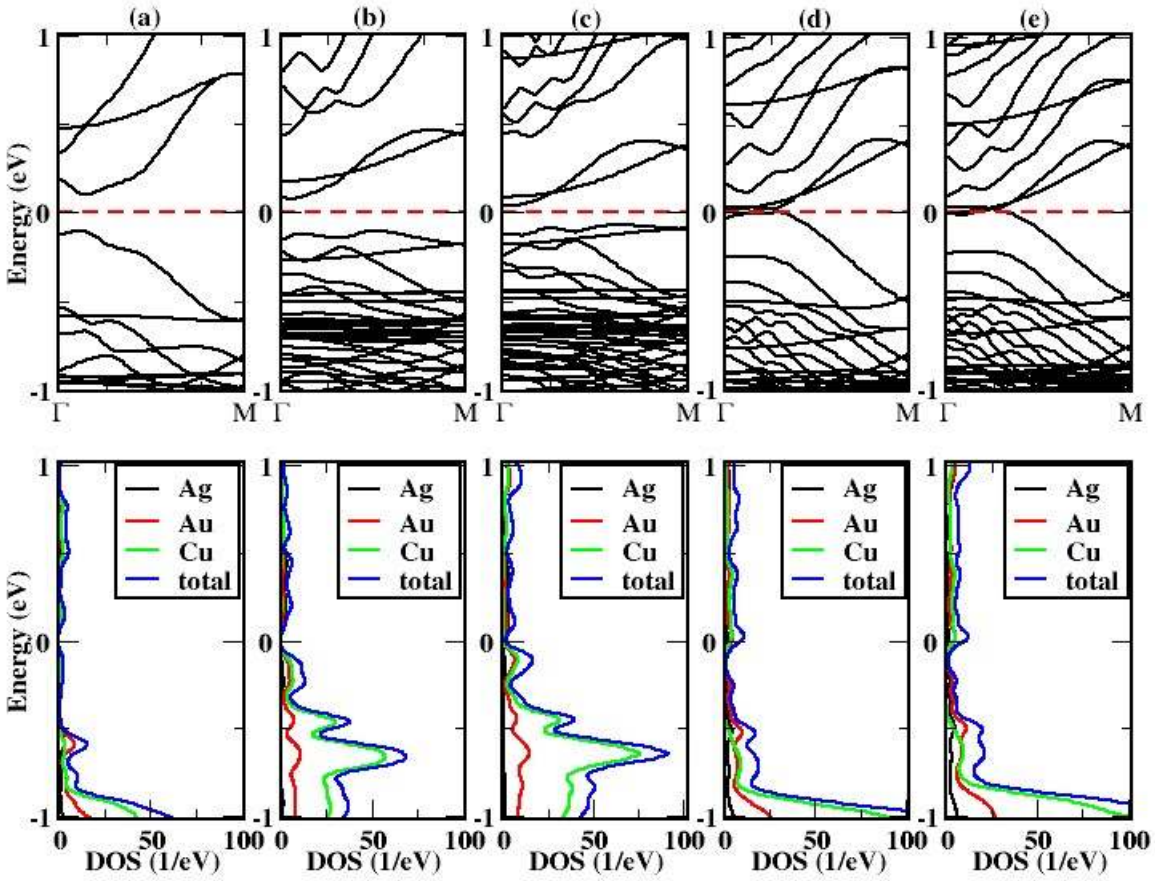
Research Challenge/s:

Since noble metal nanostructures show variation in their properties with change in their size and shape, so it would be interesting to study the structural, electronic and dielectric properties of noble metal nanotubes of different chirality and noble metal nanoribbons of different sizes.

Work carried , Milestone, Achievements & Graphs, Plots:

We are in process of finalizing our two manuscripts one on noble metal nanoribbons and other on noble metal nanotubes for publishing in journal very soon and we will inform you as soon as they get published.





Publications / Articles etc. (If any):

our two manuscripts are under ready for submisson to the journals

Awards (If any): NA

Work presented in conference/s with photographs (if any): NA

Appreciation / Recognition (if any): NA

References:

Benefits & experience of using NPSF:

The NPSF is the most well maintained resource in India. The team was always there to accommodate our querries with quick responses. We have been helped a lot during installations etc. The resource has lead to reduction in our time consumption for carrying these heavy computations.

Any other relevant information (if any):

Title of the work carried out: Stable Red Emission from Nanosheets of Molecularly Doped Hexagonal Boron Nitride

Name & Designation of the Chief Investigator: Prasenjit Ghosh, Associate Professor

E-mail Id: pghosh@iiserpune.ac.in

Institution Name: Indian Institute of Science Education and Research, Pune

Research Challenge/s:

Achieving visible photoluminescence from hexagonal boron-nitride (hBN) nanosheets is synthetically very much challenging due to its intrinsically high electronic band gap. In this work, using a combination of experimental and computational studies we have shown that this can be achieved through molecular doping. In particular, our experimental colleagues doped hBN with tetracyanoquinodimethane (TCNQ) to achieve the same. Our atomistic simulations provided a microscopic explanation of the physical process.

Work carried , Milestone, Achievements & Graphs, Plots:

We have performed ab initio based density functional theory based calculations to understand how TCNQ is doping hBN such that it emits photoluminescence at the visible region. We have considered three plausible configurations: (1) DCTC anion with a defect-free hBN layer, (2) DCTC anion with a hBN layer having nitrogen vacancy (V_N), and (3) DCTC anion with a hBN layer having boron vacancy (V_B). The defect-free hBN and DCTC anion were found to be $\sim$ 3.24 $\mathring{A}$ apart, thereby exhibiting primarily van der Waals type interaction. The density-of-state (DOS) plot showed that the contributions in the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) mainly originates from DCTC, and no defect and/or new states were observed within the gap. The interaction of DCTC with hBN (VN) was also observed to be van der Waals type and the distance between DCTC and hBN (VN) was found to be $\sim$2.93 AA an indication of a relatively stronger interaction in comparison to the former configuration. Due to intrinsic nitrogen vacancy, various defect states were observed on the DOS plot of the hBN (VN)-DCTC configuration. The probable spin-preserving transition (1.95 eV) closely matched the experimental value of $\sim$2 eV corresponding to the emission peak at 616 nm; however, the other state related to the emission at 672 nm was absent.

Finally, we have analyzed the scenario of interaction of DCTC anion with the boron vacancy (VB) in the hBN layer, which turned out to be very interesting. DCTC anion strongly interacted with boron vacancy (VB). DCTC appeared to be covalently bonded to VB, forming three CN bonds, and, as a result, the planarity of hBN was locally lifted by $\sim$1.3 AA from the plane (Figure 5a). Such a chemical activation of VB generated new electronic states (both in spin-up and spin-down channels) between the valence and the conduction band edges of hBN (Figure 5b). Among these new states, though the highest occupied state (HOMO) and the lowest unoccupied one (LUMO) are localized primarily on DCTC, they are in different spin channels, thereby making optical transitions between them impossible. However, there are two states in the spin-down channel at 1.96 and 1.8 eV that result from the hybridization of the atomic states of N of hBN-VB and the molecular orbitals of DCTC. Upon excitation, the electrons from these two states are probably transferred to the LUMO of the molecule, giving rise to transitions at $\sim$1.96 and $\sim$1.8 eV within the gap (Figure 5c), which can be assigned to the observed emission

peaks at ∼616 nm (∼2 eV) and ∼672 nm (∼1.85 eV), respectively.

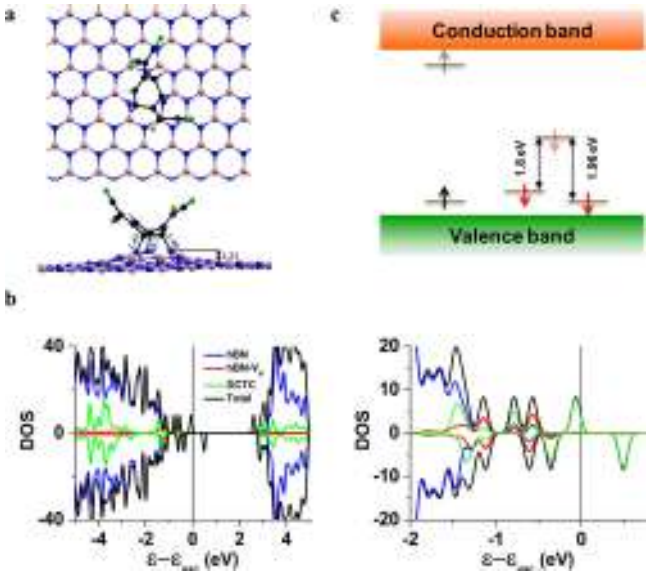


Figure 1: (a) Schematic of the energy-optimized geometry (top and side views) revealing strong interaction of DCTC with hBN-VB. (b) Total DOS plot along with the contributions of the hBN, hBN-VB, and DCTC components. A zoomed-in portion of the DOS plot is present on the right side. (c) Schematic of valence band and conduction band with possible transition states within the gap derived from the DOS plot.

Publications / Articles etc. (If any):

Stable Red Emission from Nanosheets of Molecularly Doped Hexagonal Boron Nitride, V. Kumar, N. Joshi, B. Dhara, P. Jha, S. Rana, P. Ghosh and N. Ballav, J. Phys. Chem. C, 2018, 122 (36), pp 21076-21082.

Awards (If any): NA

Work presented in conference/s with photographs (if any): NA

Appreciation / Recognition (if any): NA

References: NA

Benefits & experience of using NPSF:

Access to Param Yuva made these heavy calculations possible. I would also like to thank the staff for the excellent maintenance of the cluster (with minimal amount of downtime) and their prompt help to my students whenever they had any difficulties.

Any other relevant information (if any):

I think one needs to optimize the waiting time for a moderately sized job to start. Presently one needs to wait for days.

Title of the work carried out: Computational modeling of atomic scale systems

Name & Designation of the Chief Investigator: Dr. Puneet Kumar Patra, Assistant Professor, Department of Civil Engineering

E-mail Id: puneet.patra@civil.iitkgp.ac.in

Institution Name: Indian Institute of Technology Kharagpur

Research Challenge/s:

Computational modeling of atomic scale systems enables us to unravel interesting physics hidden underneath a complex behavior. A better understanding of such behavior can result in tailoring the properties of materials, which may find further use in real-life applications. The primary tool for computational modeling of atomic scale systems employed by us is molecular dynamics simulations. However, molecular dynamics simulations not only require large computational resources but also rationalizing the simulation techniques.

Work carried / Milestone / Achievements:

1. Understanding modal energy partition during thermal conduction in one-dimensional chains: Non-equilibrium molecular dynamics simulations have been performed to understand modal energy partition during thermal conduction in one-dimensional chains. Thermal conduction has been engineered in the chain by keeping its two ends at different temperatures. Energy of each normal mode of vibration is monitored every time step to identify the salient features of energy transport.

2. Frictional characteristics of nanotubes driven by force and torque: Constant temperature molecular dynamics simulations have been performed to identify the frictional characteristics of nanotubes as they are driven by an external force and torque while they move over a fixed graphene sheet. A 2-dimensional model of the problem has been developed whose results qualitatively agree with those of full scale 3-dimensional molecular dynamics simulations.

3. Molecular modeling of atomic force microscope tip: In order to identify the salient features of an atomic force microscope (AFM) exploring a nanoscale surface, molecular modeling of an AFM tip has been done.

4. Methodology for molecular modeling of Casimir Forces: A new technique is under development for modeling Casimir forces within the molecular dynamics framework.

Benefits experience of using NPSF:

Performing molecular dynamics simulations is a computationally expensive task. Execution of each of the work described above on a single processor or on a desktop machine takes several days. Using the NPSF computing facility, we have been able to reduce our run-time to a few hours to a few days, depending on the problem. The reduction in time has helped us in speeding up the work significantly. However, these days Param Yuva cluster has a long queue, and as a consequence some of the simple tasks take a long time to start running.

Any other relevant information (if any):

Queuing of tasks can be further streamlined so that separate jobs using single-processors can get queued quickly.

Title of the work carried out:

1. Effect of doping in Silicon nanowires along different crystal axis.
2. Effect of doping in Silicon/Germanium core/shell nanowires.
3. The computation of electrical, spin and thermal transport characteristics of complex nanowires.

Name & Designation of the Chief Investigator: Raman Sharma (Professor)

E-mail Id: bramans70@yahoo.co.in

Institution Name: Himachal Pradesh University

Research Challenge/s:

We are looking for the energetics of different doping atoms[1] in the a. Silicon nanowires modeled to grown along different crystal axis[2].

Work carried , Milestone, Achievements Graphs, Plots:

We were using Density functional Codes to carry out our investigations and the biggest hurdle in any DFT calculations is to find out the most equilibrium state of our model. We took Silicon nanowires a bit thicker than usual because that will serve two purposes. A) One cans easily models the derivative like core/shell wires of other Group IV elements[3], [4]. B) We can filter out the quantum effect because of the size of wire dimension[5]. This attempt made our unit cell quit bulky however, close to the real size that have been found in experimentally.

Not only relaxation of modeled Silicon nanowires along different crystal direction is being carried out but also we have relaxed few derivatives of nanowire such as core/shell Si/Ge and Ge/Si as well. The top views of different Si/Ge or Ge/Si core shell wire are shown. These relaxations are considered as massive jobs that need to take care by massive computation like NPSF. Next we can apply some post relaxation utilities that dont need much time and resources.

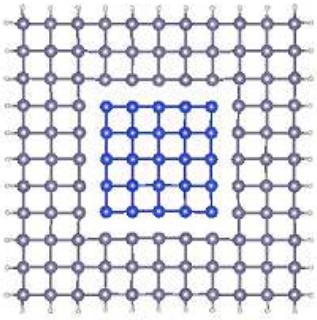


Figure 1: Top view of Germanium/Silicon core shell wire along [100] growth direction.

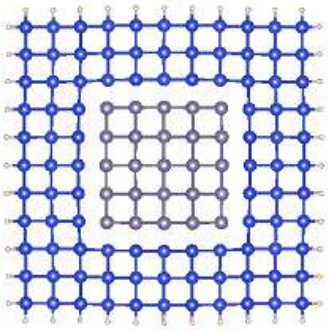


Figure 2: Top view of Silicon/Germanium core/shell wire along [100] growth direction.

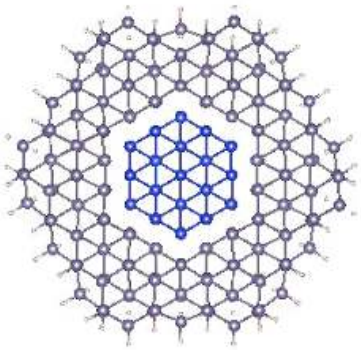


Figure 3: Top view of Germanium/Silicon core shell wire along [111] growth direction.

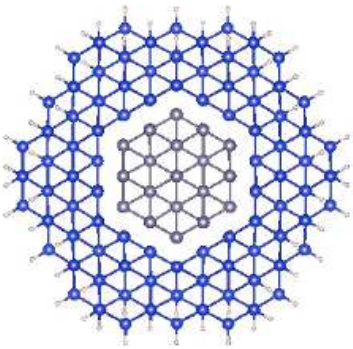


Figure 4:Top view of Silicon/Germanium core/shell wire along [111] growth direction.

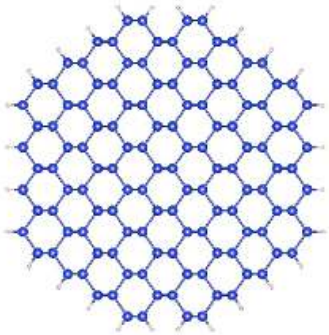


Figure 5: Top view of Silicon nanowire along [110] growth direction.

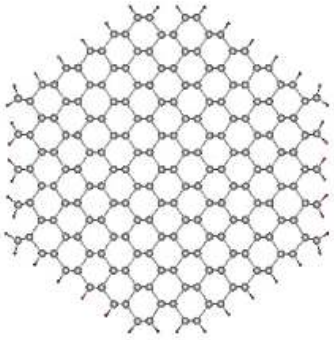


Figure 6: Top view of Germaniumnanowire along [110] growth direction.

Publications / Articles etc. (If any): Not yet.

Awards (If any): Not yet.

Work presented in conference/s with photographs (if any): Not yet.

Appreciation / Recognition (if any): Not yet.

References:

1. W. Chen et al., "Incorporation and redistribution of impurities into silicon nanowires during metal-particle-assisted growth," Nat. Commun., vol. 5, no. May, pp. 1-7, 2014.

2. Y. Tao and C. L. Degen, "Growth of magnetic nanowires along freely selectable (hkl) crystal directions," Nat. Commun., vol. 9, no. 1, pp. 1-7, 2018.

3. B. Tian et al., "Coaxial silicon nanowires as solar cells and nanoelectronic power sources," Nature, vol. 449, no. 7164, pp. 885-889, 2007.

4. D. C. Dillen, K. Kim, E. S. Liu, and E. Tutuc, "Radial modulation doping in core-shell nanowires," Nat. Nanotechnol., vol. 9, no. 2, pp. 116-120, 2014.

5. M. Nolan, S. O. Callaghan, G. Fagas, J. C. Greer, T. Frauenheim, and V. Uni, "Silicon Nanowire Band Gap Modification," 2007.

Benefits & experience of using NPSF:

Benefits: Because of massive computation one can choose the problem without taking too much concern of the massiveness of problem. We do not need to worry about the installation problem thanks to NPSF help service.

Experience: We feel delighted and obliged to NPSF for maintaining such a standard of work ethics. We feel a debt of gratitude for the services and try our best to meet NPSF team expectations.

Any other relevant information (if any):

Title of the work carried out: Numerical simulations of flow past complex bodies.

Name & Designation of the Chief Investigator: Dr. Sanjay Mittal, Professor

E-mail Id: smittal@iitk.ac.in

Institution Name: Indian Institute of Technology Kanpur

Research Challenge/s:

We employ modern stabilized finite element methods for solving the governing equations for fluid flows. Some of the flow problems arise from practical applications while others add to understanding of certain fundamental issues in fluid mechanics. Most of the applications require large scale computing. To that extent, where-ever possible, in-house codes have been parallelized using MPI libraries. Scalability on parallel computers is demonstrated. A brief overview of our work on understanding flow past bluff bodies, airfoils, wings will be presented. Some problems associated with fluid- structure interaction are also investigated. Supersonic flow inside intakes and nozzles is also studied.

Work carried , Milestone, Achievements & Graphs, Plots:

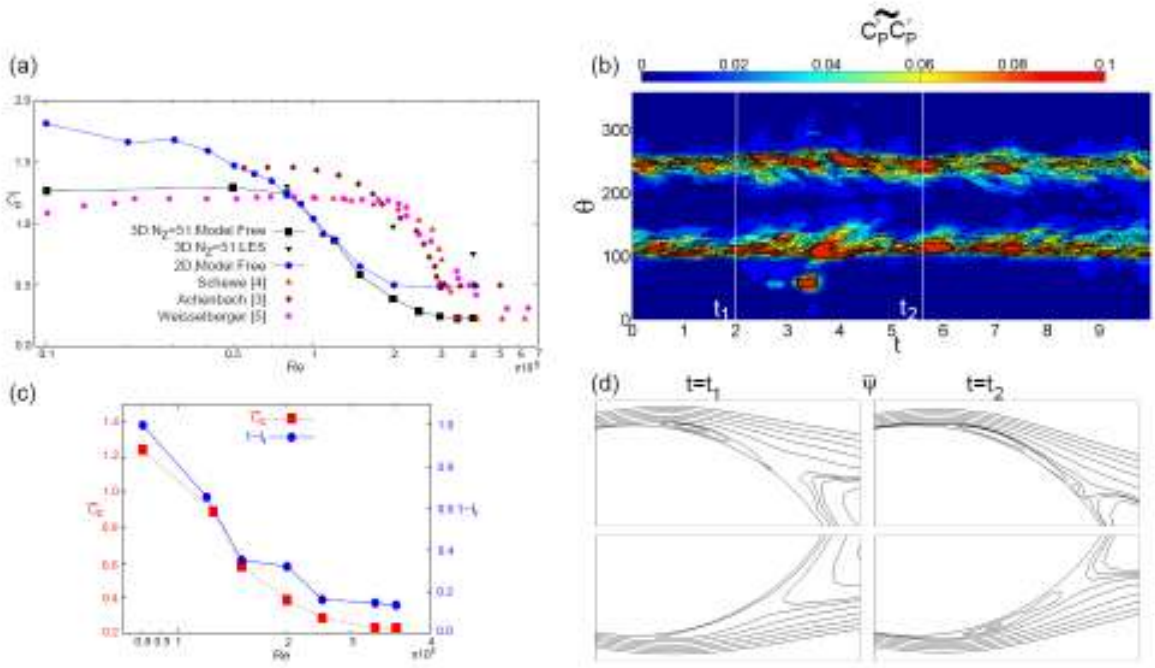


Figure 1:Flow past a cylinder: (a) variation of the mean drag coefficient with Re. Also shown are results from earlier studies. (b) Re=1.5x10^5 flow past a cylinder: space-time diagram of the rms of the fluctuations of coefficient of pressure. (c) Variation of intermittency factor with Re in solid line. Also shown in broken line in the span- and time-averaged drag coefficient. (d) Shows the close-up views of the streamlines for the span- and moving time-averaged flow at the tine instants t_1=2.0 and t_2=5.5 marked in (b).

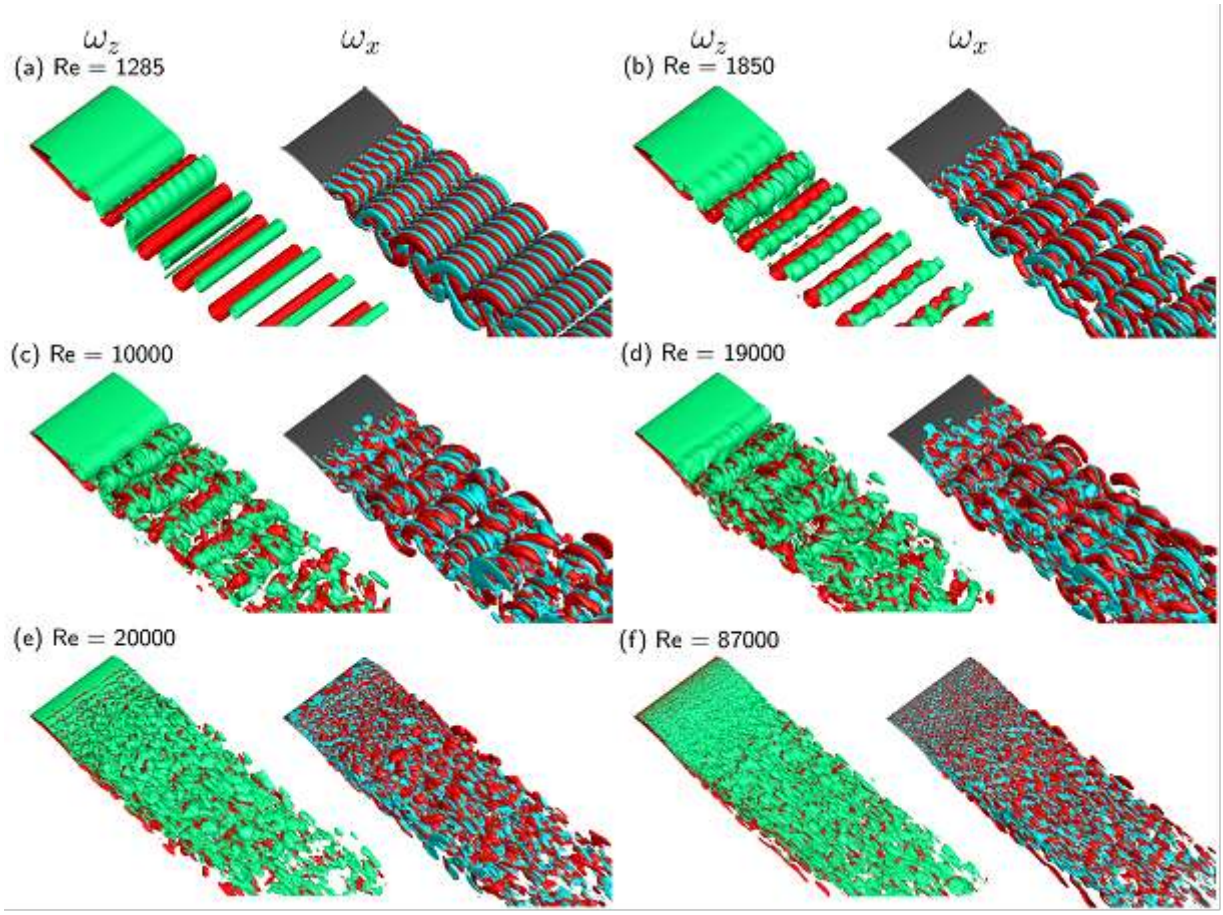


Figure 4.1: 3D Flow past an Eppler 61 airfoil at $\alpha = 10o$: iso-surfaces of spanwise ($\omega z = \pm 2$) and streamwise vorticity ($\omega x = \pm 2$) for various Re. The iso-surfaces are obtained when the instantaneous lift coefficient achieves its maximum value. The iso-surface for streamwise vorticity at Re = 1285 and 1850 is shown for $\omega x = \pm 0.01$ and $\omega x = \pm 0.5$, respectively.

Publications / Articles etc. (If any):

1. Shah, K., Shakya, R. and Mittal, S., 2019. Aerodynamic forces on projectiles used in various sports.Physics of Fluids,31(1), p.015106.

2. Chopra, G. and Mittal, S., 2019. Drag coefficient and formation length at the onset of vortex shedding.Physics of Fluids,31(1), p.013601.

3. Mittal, S. and Tezduyar, T.E., 2018. Comment on Experimental investigation of Taylor vortex photocatalytic reactor for water purification.Chemical Engineering Science,192, pp.1262-1262.

4. Deshpande, R., Shakya, R. and Mittal, S., 2018. The role of the seam in the swing of a cricket ball.Journal of Fluid Mechanics,851, pp.50-82.

5. Mittal, S. and Dwivedi, A., 2017. Local and biglobal linear stability analysis of parallel shear flows.Computer Modeling in Engineering & Sciences,113(2), pp.219-237.

6. Kotteda, V.K. and Mittal, S., 2017. Flow in a planar convergentdivergent nozzle.Shock Waves,27(3), pp.441-455.

7. Deshpande, R., Kanti, V., Desai, A. and Mittal, S., 2017. Intermittency of laminar separation bubble on a sphere during drag crisis.Journal of Fluid Mechanics,812, pp.815-840.

8. Navrose, Mittal, S., 2017. The critical mass phenomenon in vortex-induced vibration at low Re.Journal of Fluid Mechanics,820, pp.159-186.

9. Chopra, G. and Mittal, S., 2017. The intermittent nature of the laminar separation bubble on a cylinder in uniform flow.Computers & Fluids,142, pp.118-127.

Awards (If any):

Work presented in conference/s with photographs (if any):

1. Chopra, G. and Mittal, S., 2018. Large Eddy Simulation of flow past a circular cylinder in the drag crisis regime: effect of aspect ratio and the existence of multiple states.Bulletin of the American Physical Society.

2. Sahu, T.R., Chopra, G. and Mittal, S., 2018. Vortex-Induced Vibration of a Circular Cylinder at High Reynolds Numbers. International conference of Fluid Mechanics and Fluid Power.

Appreciation / Recognition (if any):

References:

Benefits & experience of using NPSF:

Any other relevant information (if any):

Title of the work carried out: Quantum transport in 2D perovskite-based Solar Cells and atomic clusters

Name & Designation of the Chief Investigator: Dr Sanjeev Kumar Gupta, Assistant Professor

E-mail Id: sanjeev.gupta@sxca.edu.in

Institution Name: St. Xavier's College, Ahmedabad, Gujarat

Research Challenge/s:

Our cost-effective and less time consuming strategy proposed in this work will assist in improving the realistic functional design of photovoltaic materials in the laboratory towards the next stage.

Work carried / Milestone/Achievements:

During the time period from January 01, 2018 till December 31, 2018, we have completed three major projects.

1. First, we have presented a thorough study of electronic and optical properties and interface charge dynamics, that revealed $CaMnO_3$ as a better candidate for the electron transport material in thin film hole transporting material free hybrid perovskite solar cells with the planar architecture than the most common anatase TiO_2.

2. Secondly, the temperature dependent switching mechanism of carbon dioxide (CO_2) molecule by alkaline earth metal (AEM) (Mg^{+2}, Ca^{+2}, Sr^{+2} and Ba^{+2}) functionalized on graphitic boron nitride (g-B4N_3) nanosheet have been analyzed by using densityfunctional theory (DFT) approach includes long-range correlation (DFT+D2). This method has been implemented in such a way to understand the switchable or capture/release mechanism of CO_2 molecule. The positive valance alkaline earth adatoms on the nanosheet of g-B4N_3 has been provided external energy to do the capture/release process of greenhouse gas CO_2. Due to the weak adsorption of CO_2, it makes possible to discharge from the g-B4N_3 nanosheet and shows instantaneous switching mechanism. Briefly, the negatively charged g-B4N_3 nanosheets are highly sensitive for CO_2.

3. And recently, we have studied the structural, electronic and optical properties of single-layer carbon phosphide (CP) allotropes (a-, b- and c-phases) based on density functional theory. The thermoelectric properties like electrical conductivity, thermal conductivity, thermo-electric power, figure of merit (ZT) and compatibility factor as a function of temperature are calculated by using BoltzTrap code. The electronic band structures reveal the direct band gap of a- and b-CP monolayer (i.e., semiconducting nature), while c-CP monolayer is semimetallic with Dirac fermions. The significant absorption is observed in a-, b- and c-CP monolayer, which can be used as an ultraviolet opticalnanodevice, and all three phases of monolayer of CP are directionally transparent. The transmission spectrum of monolayer of b- and c-phase in the visible region is much higher; therefore, it is used in an anti-reflecting layer in solar cell also. The a-phase of CP monolayer in the ZT increases linearly up to 1500 K, and beyond it reached maximum values as compared to other phases. The results show that below 550 K, CP allotropes (both n- and p-types) are hitherto the best-promising

thermoelectric materials. These theoretical investigations suggest that the different phases of semiconducting materials of CP are better candidate for potential application in micro-/nanoscale device, photovoltaic and optoelectronics.

4. The 2D halide perovskite have distinct modulate compositional and structural tunable properties, which makes 2D materials as good candidate to improve the characteristics of photovoltaic applications. We have explored strain dependent structural, electronic and optical properties of organicinorganic hybrid perovskite CH3NH3PbI3 monolayer using the density functional calculations. Here, we have calculated carrier mobility and band gap of CH3NH3PbI3 monolayer. The results suggest that with increasing tensile and compressive strain, the band gap increases up to 5% (in tensile), while decreases towards instability i.e. 9% of compressive strain. The carrier mobility of 2D CH3NH3PbI3 is approximately 16 times larger than bulk form of CH3NH3PbI3.

Publications / Articles etc. (If any):

1. Kansara, S., Gupta, S. K., Sonvane, Y., & Srivastava, A. (2018). Switching mechanism of CO_2 by alkaline earth atoms decorated on g-$B4N_3$ nanosheet. arXiv preprint arXiv:1805.11283.

2. Singh, D., Kansara, S., Gupta, S. K., & Sonvane, Y. (2018). Single layer of carbon phosphide as an efficient material for optoelectronic devices. Journal of materials science, 53(11), 8314-8327.

3. Singh, D., Singh, N., Gupta, S. K., & Sonvane, Y. (2018, April). Effect on electronic and optical properties of Frenkel and Schottky defects in HfS2 monolayer. In AIP Conference Proceedings (Vol. 1942, No. 1, p. 090023). AIP Publishing.

4. Pandey, K., Singh, D., Gupta, S. K., Yadav, P., Sonvane, Y., Lukaevi, I., ... & Ahuja, R. (2018). Improving electron transport in the hybrid perovskite solar cells using CaMnO3-based buffer layer. Nano Energy, 45, 287-297.

5. Sandip R. Kumavat,Yogesh Sonvane,Deobrat Singh, andSanjeevK.Gupta, Two-Dimensional CH3NH3PbI3with High Efficiency and Superior Carrier Mobility: A Theoretical Study, J. Phys. Chem. C,2019,123(9),pp 52315239.

Awards (If any):

Best Research Paper award in Physical Science by Gujarat Science Academy (GSA).

Appreciation / Recognition (if any):

Received award and citation **Researcher of the year 2018** for the outstanding contribution in the field of physics, St. Xaviers College, Ahmedabad, Gujarat.

References:

1. Singh, D., Kansara, S., Gupta, S. K., & Sonvane, Y. (2018). Single layer of carbon phosphide as an efficient material for optoelectronic devices. Journal of materials science, 53(11), 8314-8327.

2. Singh, D., Singh, N., Gupta, S. K., & Sonvane, Y. (2018, April). Effect on electronic and optical properties of Frenkel and Schottky defects in HfS2 monolayer. In AIP Conference Proceedings (Vol. 1942, No. 1, p. 090023). AIP Publishing.

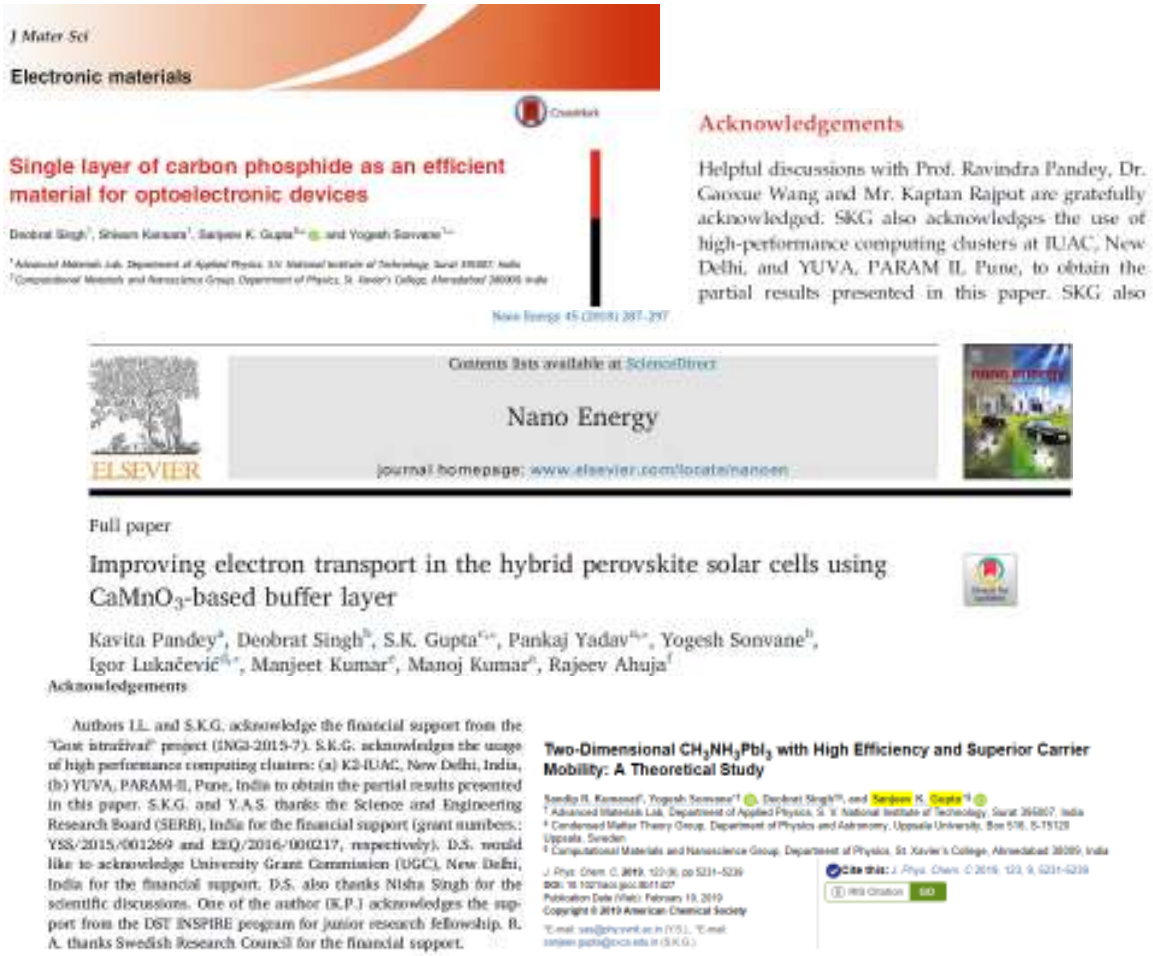
3. Pandey, K., Singh, D., Gupta, S. K., Yadav, P., Sonvane, Y., Lukaevi, I., ... & Ahuja, R. (2018). Improving electron transport in the hybrid perovskite solar cells using CaMnO3-based buffer layer. Nano Energy, 45, 287-297.

4. Sandip R. Kumavat,Yogesh Sonvane,Deobrat Singh, andSanjeevK.Gupta, Two-Dimensional CH3NH3PbI3with High Efficiency and Superior Carrier Mobility: A Theoretical Study, J. Phys. Chem. C,2019,123(9),pp 52315239.

Benefits & experience of using PARAM Yuva II:

The proposed work is one of the important directions both in the fundamental and applied sciences. In addition, the outcome will be beneficial for the research students participating in the projects giving them opportunity to perform scientific investigation at national/international level and to meet and discuss with scientist and students from other international laboratory. This supercomputing collaboration can also be extended for the future. It is expected that the studies performed will lead to publications in refereed international journals and will be suitable for presentation at local and international conferences.

Any other relevant information (if any):



J Mater Sci

Electronic materials

Single layer of carbon phosphide as an efficient material for optoelectronic devices

Acknowledgements

Helpful discussions with Prof. Ravindra Pandey, Dr. Caoxue Wang and Mr. Kaptan Rajput are gratefully acknowledged. SKG also acknowledges the use of high-performance computing clusters at IUAC, New Delhi, and YUVA, PARAM II, Pune, to obtain the partial results presented in this paper. SKG also

Contents lists available at ScienceDirect

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journal homepage: www.elsevier.com/locate/nanoen

Full paper

Improving electron transport in the hybrid perovskite solar cells using $CaMnO_3$-based buffer layer

Kavita Pandey, Deobrat Singh, S.K. Gupta, Pankaj Yadav, Yogesh Sonvane, Igor Lukačević, Manjeet Kumar, Manoj Kumar, Rajeev Ahuja

Acknowledgements

Authors I.L. and S.K.G. acknowledge the financial support from the "Gost istraživač" project (INGI-2015-7). S.K.G. acknowledges the usage of high performance computing clusters: (a) K2-IUAC, New Delhi, India, (b) YUVA, PARAM-II, Pune, India to obtain the partial results presented in this paper. S.K.G. and Y.A.S. thanks the Science and Engineering Research Board (SERB), India for the financial support (grant numbers.: YSS/2015/001269 and EEQ/2016/000217, respectively). D.S. would like to acknowledge University Grant Commission (UGC), New Delhi, India for the financial support. D.S. also thanks Nisha Singh for the scientific discussions. One of the author (K.P.) acknowledges the support from the DST INSPIRE program for junior research fellowship. R. A. thanks Swedish Research Council for the financial support.

Two-Dimensional $CH_3NH_3PbI_3$ with High Efficiency and Superior Carrier Mobility: A Theoretical Study

Computational facilities from the Center for Development of Advance Computing (C-DAC) Pune are also gratefully acknowledged.

Title of the work carried out: Three dimensional modelling of Magnetotelluric Data over Dalma and Dhanjori Volcanics.

Name & Designation of the Chief Investigator: Prof. Shalivahan (Dean R&D, IIT(ISM), Dhanbad)

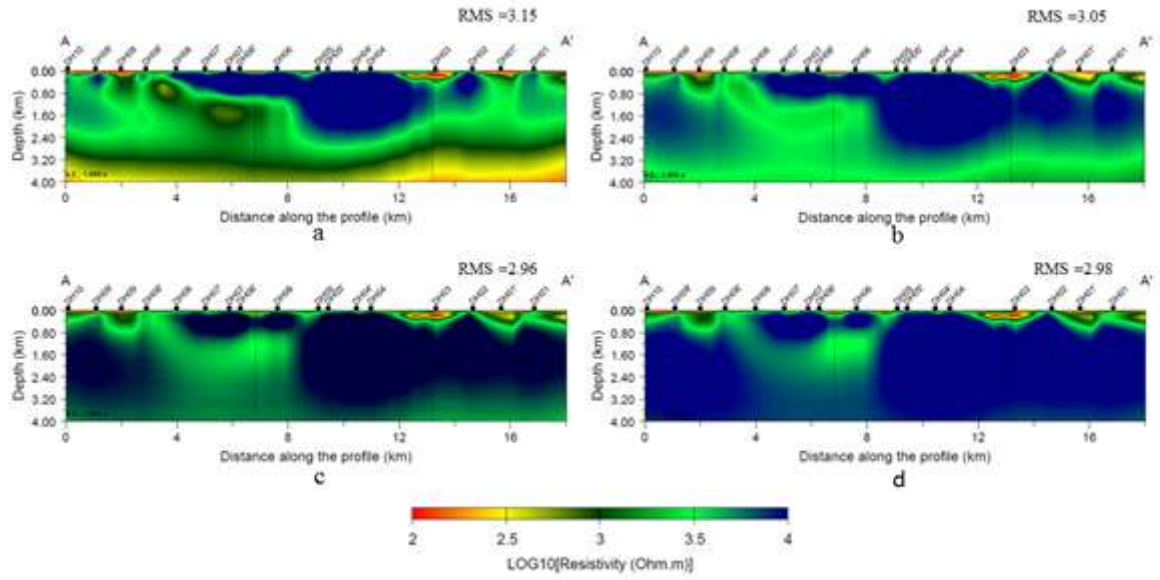
E-mail Id: shalivahan@iitism.ac.in

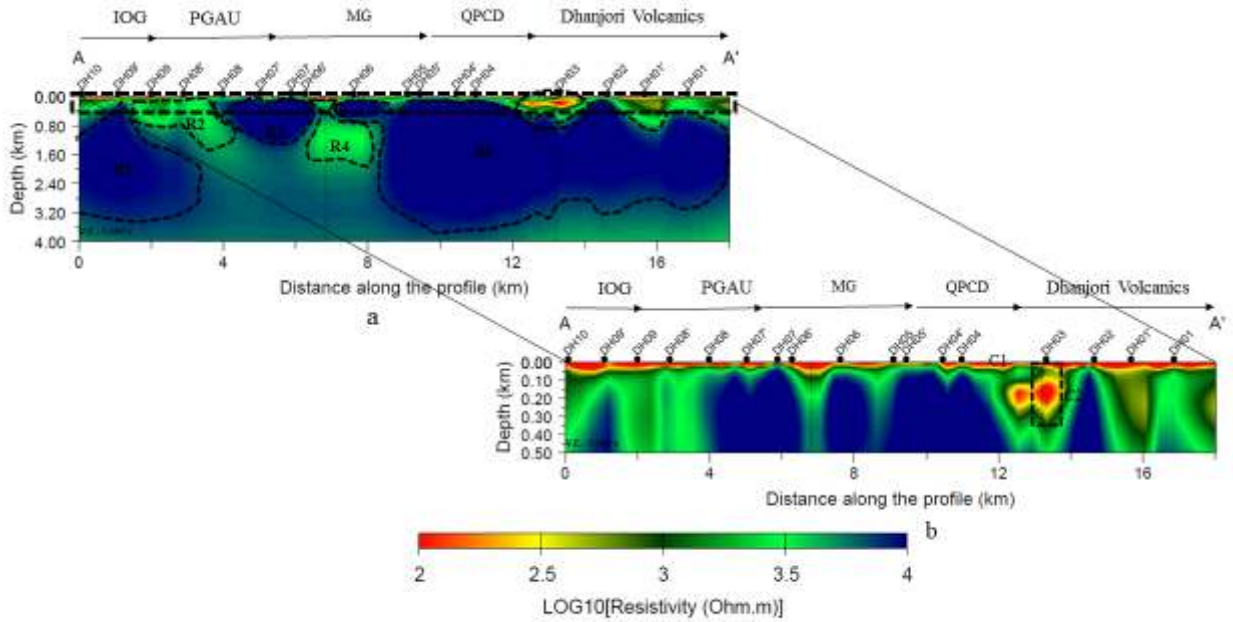
Institution Name: Indian Institute of Technology (ISM), Dhanbad

Research Challenge/s:
Working with the project the availability of high computational facility was always a challenge among the other challenge. The work demanded a system with a high computation speed with all the necessary libraries and the operating system where all the softwares and the codes could run and also stores large output.

Work carried , Milestone, Achievements & Graphs, Plots:

3D inversion results





Publications / Articles etc. (If any):

1. Singh, Roshan & Maurya, Ved & Ss, Shalivahan & Singh, Sahendra. (2019). Imaging Regional Geology and Au - Sulphide mineralization over Dhanjori greenstone belt: Implications from 3-D Inversion of Audio Magnetotelluric data and Petrophysical Characterization. Ore Geology Reviews. 10.1016/j.oregeorev.2019.01.027

2. Singh, R.K., Gupta, A.K., Maurya, V.P., Singh, S., Shalivahan, 2019. 3D Inversion of Audio Magnetotelluric data for sulphide mineralization over Dhanjori Basin. Geological Society of India p. 213-217, ISSN 0974-6889.

Awards (If any):

Work presented in conference/s with photographs (if any):

Presented work in Emerging Trends in Geophysical Research for Make in India (ETGRMI) 9-11 March, 2018, IIT(ISM) Dhanbad on the occasion of the Diamond Jubilee Celebration organized by Department of Applied Geophysics

Appreciation / Recognition (if any):

References:

Benefits & experience of using NPSF:

3D inversion of Magnetotelluric data is computationally very intensive. Using NPSF significantly reduced the inversion time. Before concluding to a final model one is required to test many parameters and running the inversion a number of times which is also very much time consuming. We had a very pleasant experience using NPSF where we were given enough of memory as well as in most if the cases the queue time was not very large. And the support which we got over the years were very good. The support staffs always helped and they were very soft.

Any other relevant information (if any):

Title of the work carried out:

1. Exploring turbulence and fluctuation dynamos in galaxies and clusters (by Sharanya Sur)
2. Magnetic reconnection forced by MHD waves in the solar corona (by Piyali ChaHerjee)

Name & Designation of the Chief Investigator:

Sharanya Sur, Reader
Piyali ChaHerjee, Reader (Co-Investigator)

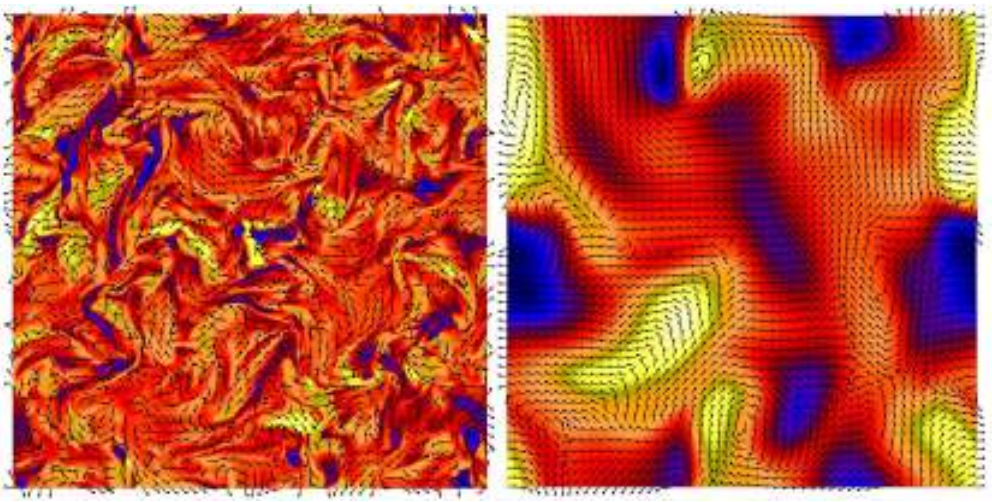
E-mail Id: sharanya.sur@iiap.res.in, piyali.chaHerjee@iiap.res.in

Institution Name: Indian Institution of Astrophysics, Bangalore

Research Challenge/s:

Work carried , Milestone, Achievements & Graphs, Plots:

1. Decaying turbulence and magnetic fields in galaxy clusters - studying the decay of turbulence and Fluctuation dynamo generated magnetic fields in galaxy clusters. Fig. 1 shows the time evolution of the dynamo generated field in saturated (leY) and decaying (right) phases.



   The fields are strong in the blue and yellow regions and negligible in the orange regions. The arrows denote the direction of the field in the plane of the slices.

2. An important observational signature of fluctuation dynamos in young galaxies and clusters is the Faraday rotation measure (RM) which probes the magnetic field along the line of sight. Other than the Faraday RM, the other directly observable quantities of interest are the synchrotron emissivity and polarization signals. We are currently exploring how fluctuation dynamo simulations can be used to quantify and extract emissivity and polarization signals.

3. We carried out several tests on our 2D radiative Magneto-hydrodynamic simulation of a realistic solar atmosphere from subsurface to photosphere, chromosphere, transition region

and corona. The domain extends from -10 Mm below solar surface to 25 Mm above. The grid size is 48 km on the solar surface resolved by 768X768 grid points in x-z plane. The numerical challenges in the solar corona are mainly due to very high Alfven speeds (or low Plasma beta parameter) and very high and anisotropic thermal conductivity along magnetic field lines. To circumvent the same, we used a semi-relativistic Boris correction and used a hyperbolic heat transport equation akin to the Telegraphic

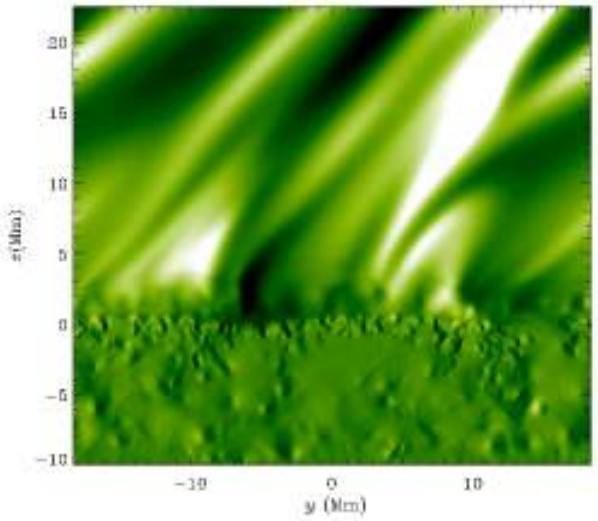


Figure 4.2: A colored contour plot of the computational domain showing the vertical velocity (km/s). The dark(white) shade corresponds to -10 (+10) km/s. The subsurface convection zone can be easily discerned from the rest of the solar atmosphere - chromosphere, transition region and the corona due to presence of convective plumes. The contours are aligned along the constant (in space) but tilted magnetic field lines of strength 7 Gauss.

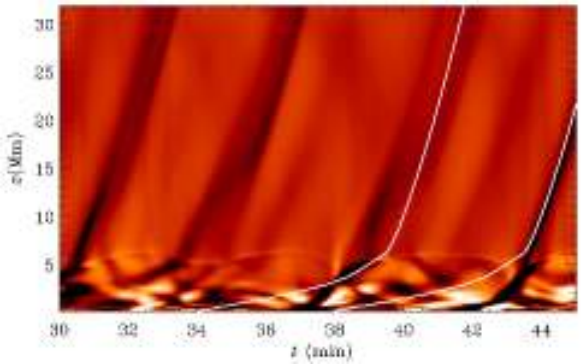


Figure 4.3: A height-time plot of the divergence of velocity representing compression (black) & rarefaction (white) for a sequence of snapshots like that in FIG 1 computed by looking through a narrow slit aligned along the tilted magnetic field lines. We clearly see propagation of slow magneto acoustic waves with the speed of sound (the slope of the solid white line aligned with the compression region).

equation. We used the open source pencil code for this purpose. We successfully ran several tests to check for fast/slow magneto acoustic wave propagation. Then in order to avoid reflection of the waves as the top boundary (in the solar corona), we included a sponge layer to absorb the velocity and magnetic field perturbations. We also made sure that the dissipation in the sponge layer does not add back to the energy equation. Then we experimented with several magnetic field topologies in the solar corona including constant

tilted magnetic field as well as a dipolar and quadrupole configurations. These will serve as wave guides for the fast and slow magneto- acoustic waves. Note, that the Alfven wave is eliminated as it cannot exist in a 2D atmosphere. These MHD waves are produced by the subsurface convection which jiggle the magnetic field lines in the solar atmosphere which are actually tethered inside the sun. Further, we modify the background magnetic field from a constant tilted topology with strength 1 G everywhere to a dipolar as well as a quadrupole potential field topology with magnetic field strength at the photosphere being around 600 G. We find an interesting phenomena not seen in any other simulations known in the literature of MHD waves, namely forced magnetic reconnection due to MHD waves. We illustrate the phenomena below for a quadrupole potential field morphology. Most of this work is under progress. Just to provide a benchmark, these simulations require at least 512 cores on sandy bridge processors on Param Yuva-II but only 128 broadwell processors on our local HPC Nova@IIA. However, we do not have the capacity to scale it to a 3D simulation on Nova@IIA (which we are testing now nevertheless) and soon will have to take a recourse to CDAC Param Yuva.

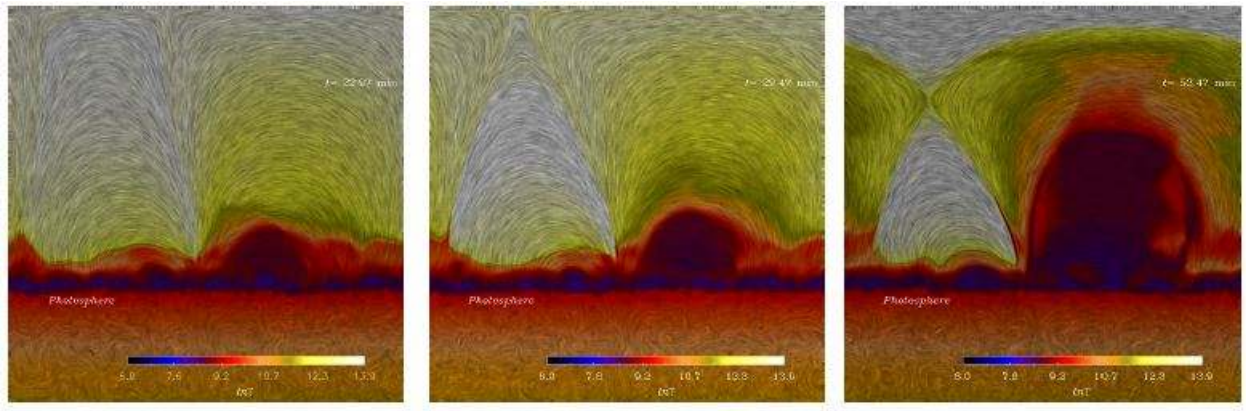


Figure 4.4: From left to right : Snapshots of the domain (X-Z plane) at three different times in increasing order showing the vector magnetic field (drawn using a line integration convolution method available as a suite MGLIB for IDL). The shaded are contours of log T according to the colorbar. In the middle panel we clearly see one of the magnetic arcade being compressed by the other one leading to heating. In the bottom panel we see a X point reconnection appearing due to a non linear stage of this arcade compression and high temperature due to the Ohmic losses in the reconnection region.

Publictiaons / Articles etc. (If any):

1. Decaying turbulence and magnetic fields in galaxy clusters, Sur, Sharanya, 2018, MNRAS (submiHed).

2. Faraday rotation from magnetic fields in young galaxies, Sur, Sharanya, Astronomy in Focus, International Astronomical Union, 2019 (in press).

3. Applying the weighted horizontal magnetic gradient method to a simulated flaring Active Region, Korsos, M., ChaKerjee, P. & Erdelyi, R. 2018, ApJ, 857, 103 DOI: 10.3847/1538-4357/ aab891 (arXiv:1804.10351)

4. Testing Alfven wave propagation in a realistic set-up of the solar atmosphere", ChaKerjee, P. 2018, GAFD (submiHed) (arXiv:1806.08166)

Awards (If any):

Work presented in conference/s with photographs (if any):

Work presented by Sharanya Sur :

1. Faraday rotation from magnetic fields in young galaxies - Focus meeting 8 on New Insights in Extragalactic magnetic fields, 30th General Assembly of the International Astronomical Union, Vienna, 2018.
2. Faraday rotation signatures of Fluctuation dynamos in young galaxies - Astrophysics colloquium, Georg August University, Goenngen, Germany, Sept. 2018.
3. Faraday rotation signatures of Fluctuation dynamos in young galaxies - Institute seminar, Hamburger Sternwarte, Hamburg, Germany, Sept. 2018.

Work presented by Dr. Piyali ChaKerjee :

4. Conference on Plasma Simulations Department of Physics, Indian Institute of Science, January 18-19, 2018.

Appreciation / Recognition (if any):

References:

Benefits & experience of using NPSF:

1. Param Yuva II has so far been extremely useful for running high resolution (512^3 and above) of MHD turbulence using up to 1024 cores. We hope that the waiting time in the queue for these demanding simulations can be further shortened.
2. It has been observed that jobs keep crashing due to node issues severely impacting the smooth running of jobs and causing a delay in timely execution of runs. Although such unforced errors may happen, it will only help the end user if efforts are taken promptly to address and minimize such issues from occurring. In such an event, the user who job failed due to node issues could be allowed to run his/her job on a priority basis to make up for the lost time.
3. For 2D runs, we tested our code successfully on Param Yuva. Scaling this to 3D will require us to use Param Yuva more frequently for cores ¿ 2048. In the testing phase the queueing time has improved over last year but is still quite long. However for high cadence output (due to sampling Nyquist criteria), the data transfer to our local computers for analysis is still a problem because of transfer speeds and unavailability of scratch space on Param. We think these issues decreasing the efficiency of the work being carried out.

Any other relevant information (if any): None.

Title of the work carried out: Molecular Dynamics Simulations on EngA : Conformational Studies

Name & Designation of the Chief Investigator: Dr. S Krishnaveni, Assistant professor, Department of Studies in Physics, Manasagangotri, Mysuru-57006

E-mail Id: sk@physics.uni-mysore.ac.in

Institution Name: University of Mysore

Research Challenge/s:

EngA(Essential neisserial GTPase A) is a GTPase (GTP binding protein) involved in Ribosome biogenesis i.e., mutation or depletion of EngA results in incomplete formation of ribosome. But it is still challenging to understand, how EngA functions at the molecular level in ribosome biogenesis (assembling ribosome RNAs and ribosome proteins into functional ribosome). It is reported in the literature that conformational states of EngA dictates EngA to bind with ribosome and facilitates in ribosome biogenesis. Therefore we are attempting to understand the conformational transitions of EngA using molecular dynamics (MD) simulations.

Work carried:

We have conducted MD simulations of EngA for the existing crystal structures of Bacillus subtilis and Thermotoga maritima species in order to understand the confomational transition pathway. Our simulations exhibits local conformational changes, which are the initiative steps for the complete transition pathway. We still have to find out the complete transition pathway and stability at the different meta states in the intermediate pathway.

Conferences:

We are presenting our simulation results in the two conferences, which are given in the following list:

1. "Molecular Dynamics Simulations on EngA A GTPase involved in Ribosome Assembly " for the conference on "Advanced Functional Materials for Energy, Environment and Health Care" at Vijnana Bhavan, University of Mysore from Mar 18-20,2019.
2. "Conformational Studies on EngA GTPase using Molecular Dynamics Simulations" for the National Seminar on Biomolecular structure and dynamics (BSAD 2019) at Periyar University from March 28-29, 2019.

Appreciation:

We are very much happy with the NPSF help desk, They respond immediately for all our queries and help in all technical issues. We hope that this help continues to solve our forthcoming issues in carrying out our simulation work.

References:

1. Robinson, V. L., Hwang, J., Fox, E., Inouye, M., Stock, A. M. (2002). Domain arrangement of Der, a switch protein containing two GTPase domains. Structure, 10(12), 1649-1658.

2. Muench, S. P., Xu, L., Sedelnikova, S. E., Rice, D. W. (2006). The essential GTPase YphC displays a major domain rearrangement associated with nucleotide binding. Proceedings of the National Academy of Sciences, 103(33), 12359-12364.

3. Majumdar, S., Acharya, A., Tomar, S. K., Prakash, B. (2017). Disrupting domain-domain interactions is indispensable for EngA-ribosome interactions. Biochimica et Biophysica Acta (BBA)-Proteins and Proteomics, 1865(3), 289-303.

Benefits experience of using NPSF:

We started using NPSF facility since July 2018, from that time NPSF system admins are very supportive and encouraging by solving all technical issues. We are happy and want to conduct more advanced MD simulations in order to find out solutions to our scientific questions of interest.

Title of the work carried out: Unconventional phase transition in classical cubic dimer model

Name & Designation of the Chief Investigator: Sreejith G J

E-mail Id: sreejith@iiserpune.ac.in

Institution Name: IISER Pune

Research Challenge/s:

Demonstrate using large scale Monte Carlo simulations that there is a hidden emergent symmetry at the critical point in a simple model of classical dimers, which is related to a phase transition in quantum spin systems.

Work carried , Milestone, Achievements & Graphs, Plots:

Please see the published article

Publications / Articles etc. (If any):

- Emergent SO(5) symmetry at the columnar ordering transition in the classical cubic dimer model, Sreejith G J, S Powell, A Nahum Physical Review Letters (Accepted; To appear in Feb/March 2019) eprint: https://arxiv.org/abs/1803.11218

Benefits experience of using NPSF:

Thank you for providing the resources. The resources provided by NPSF has been acknowledged in the published article. Some hopefully useful feedback on my experience using the service: The actual available resources were significantly less than what was allocated and availability was extremely unpredictable. It might be better to promise a more realistic number of processor hours. It might be useful to benchmark the resources provided with that in international research institutes. The login procedure was painful. It prevented accessing the files through sftp from Linux browsers. Blocking of server access from outside a limited set of ip addresses meant that we could not submit jobs when traveling or when working from home. Perhaps these can be improved.

Any other relevant information (if any):

Title of the work carried out: New structural insights into unusual nucleic acid conformations in relevance to mechanisms and pathogeneses of trinucleotide repeat expansion disorders

Name & Designation of the Chief Investigator: Thenmalarchelvi Rathinavelan

E-mail Id: tr@iith.ac.in

Institution Name: Indian institute of Technology Hyderabad

Research Challenge/s:

Trinucleotide repeats belong to the family of microsatellites (a tract of 1 to 6 repetitive nucleotides) that are commonly observed in eukaryotes and exhibit repeat length polymorphism The inherent ability of trinucleotide repeats to undergo abnormal expansion (viz. increase in repeat length) leads to many incurable genetic disorders, the best known are, Huntington's disease (CAG repeat), fragile X syndrome (CGG repeat), myotonic dystrophy 1 (CTG repeat), Friedreichs ataxia (GAA repeat) and spinocerebellar ataxias (CAG repeat) that are mainly neurodegenerative (Usdin, 2008, Krzyzosiak et al., 2012, La Spada and Taylor, 2010, Kozlowski et al., 2010a, Kozlowski et al., 2010b). Severity of these disorders is proportional to the number of expanded repeats. Overexpansion of these repeats results in the formation of unusual nucleic acid secondary structures such as hairpins, triplexes, tetraplexes etc (Mirkin, 2007). Although many investigations are being carried out to understand the mechanism(s) behind these disorders, the therapeutics of trinucleotide repeat expansion disorders are not well developed. Thus, to facilitate the therapeutics of aforementioned neurological and neuromuscular disorders, impact of such an overexpansion on DNA & RNA conformations and the concomitant functional implications have to be investigated.

Work carried , Milestone, Achievements & Graphs, Plots:

Non canonical A...A mismatch in CAG base pairs induces B to Z DNA conformation Molecular dynamics simulations on DNA hairpin stems containing A...A mismatches in a CAG repeat overexpansion show that A...A dictates local Z-form irrespective of starting glycosyl conformation, in sharp contrast to canonical DNA duplex. Transition from B to Z is due to the mechanistic effect that originates from its pronounced structural dissimilarity with flanking canonical C...G&G...C base pairs facilitated by base extrusion, backbone and/or base flipping (Figure 1) (Khan et al., 2015). Based on these structural insights we envisage that such an unusual DNA structure of the CAG hairpin stem may have a role in disease pathogenesis by binding with Z-DNA specific proteins. As this is the first study that delineates the influence of a single A...A mismatch in reversing DNA helicity, it would further have an impact on understanding DNA mismatch repair.

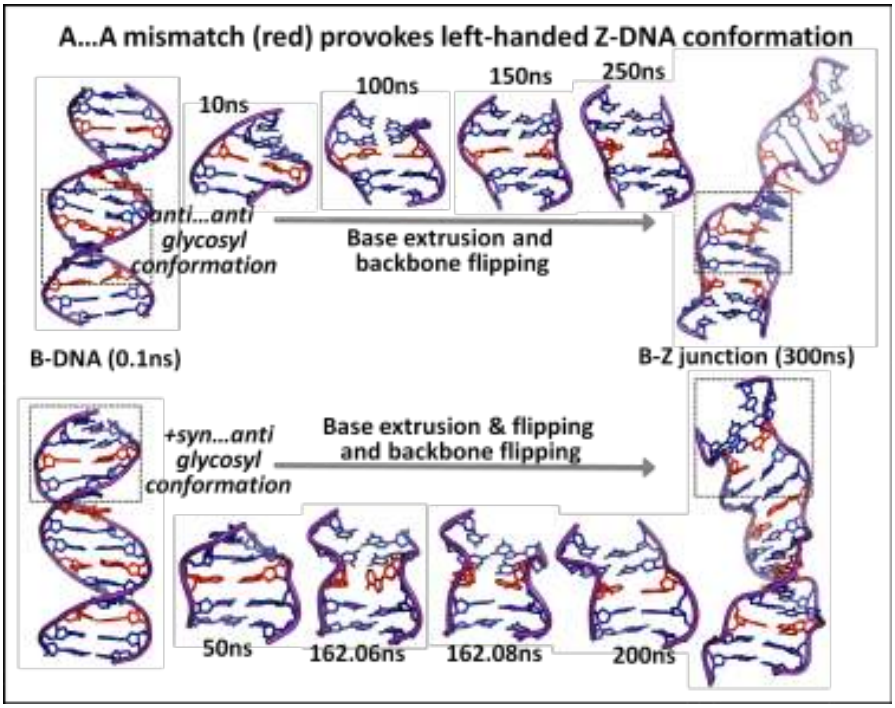


Figure 1. Evolution of B-Z junction in d(CAG)6.d(CAG)6 duplex with anti...anti and +syn...anti starting glycosyl conformations for A...A mismatch.

A...A mismatch in GAC base pairs imposes B-Z junction formation Effect of A...A mismatch in d(GAC)6.d(GAC)6 duplex has been investigated at the atomistic level using molecular dynamics (MD) simulations by considering two different starting glycosyl conformations for the mismatch following the earlier studies (Yildirim et al., 2013, Khan et al., 2015). In one model, both As are chosen to have anti glycosyl conformation. One of the two As in the second model is chosen to be in anti glycosyl conformation and the second one is chosen to be +syn glycosyl conformation. Similarly, Gs that are engaged in canonical hydrogen bonding with Cs profoundly favor -syn/+syn glycosyl conformation.

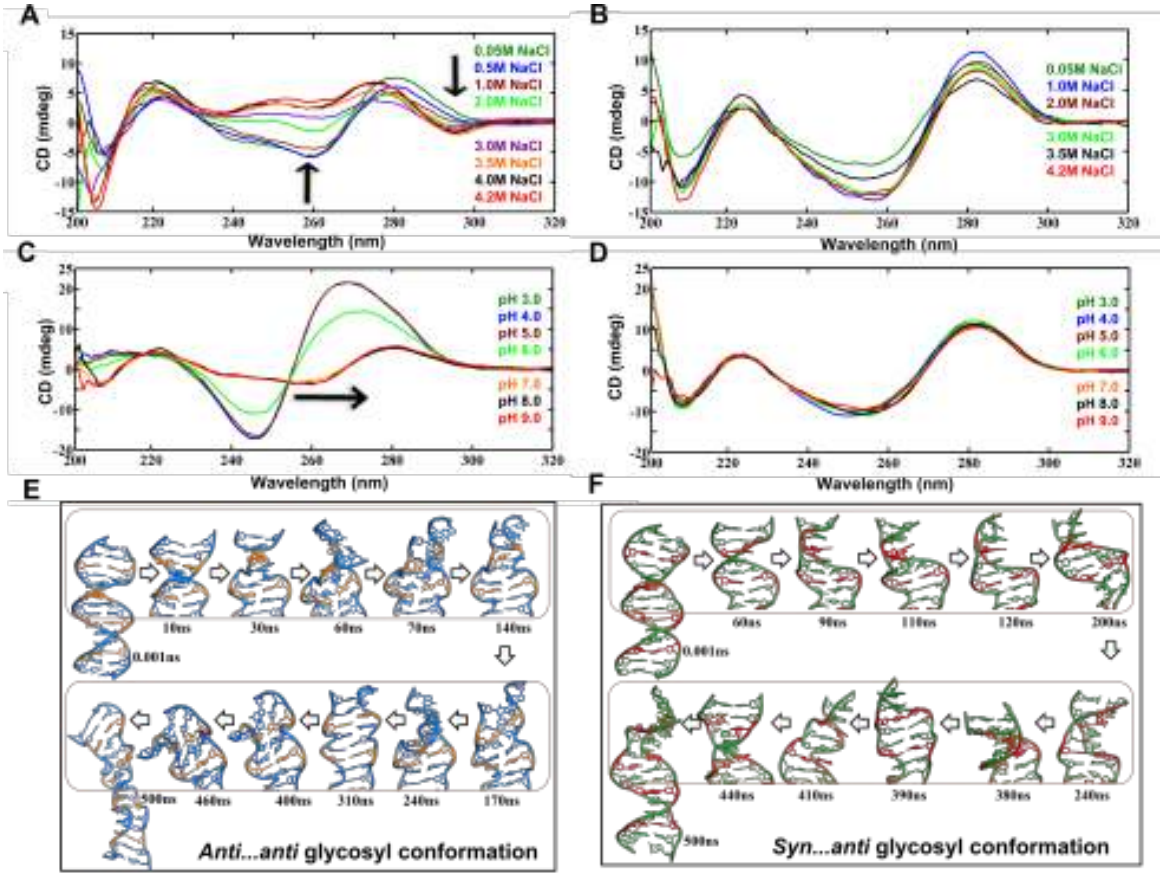


Figure 2. CD spectra and MD simulations showing the role of AA mismatch in promoting Z-phillicity in d(GAC)n.d(GAC)n duplex. Salt dependent (A) B-to-Z transition in d(GAC)5.d(GAC)5 containing canonical A...A mismatch and (B) absence of the same in d(GAC)5.d(GTC)5 containing canonical base pairs can be seen. pH induced (C) parallel duplex formation in d(GAC)5.d(GAC)5 and (D) retention of B-form in d(GAC)5.d(GTC)5 duplex. Snapshots of GAC DNA duplex during 500ns simulation indicating the formation of left-handed conformation irrespective of initial (E) anti...anti and (F) syn...anti glycosyl conformations.

GAC repeats containing A...A mismatches show local B to Z DNA transition associated with pseudoachondroplasia. In contrast, canonical base pairs retain initial B-form geometry. Circular dichroism studies further corroborate a local B- to Z in GAC repeat containing DNA duplex. Thus, the results illustrated that non canonical A...A mismatch have similar impact on DNA duplexes containing GAC & CAG repeats.

C...C mismatches distort CCG RNA duplex whereas in DNA retained B-form geometry Overexpansion of CCG repeats cause unusual secondary structures in DNA as well as in RNA. This leads to genetic instability and causes fragile XE syndrome. To investigate the stability of secondary structure in CCG repeats containing C...C mismatches, we have carried out molecular dynamics simulation and circular dichroism methods. Our investigation showed for the first time that CCG repeats containing more than four C...C mismatches in RNA are prone to form i-motif like structures, that are intolerance to form hairpin. In contrast, four C...C mismatches or below in CCG repeats are stabilized by forming hairpin or duplex structure (Figure 3.1), whereas, DNA is very stable even at six C...C mismatches and forms a stable duplex structure (Figure 3.2).

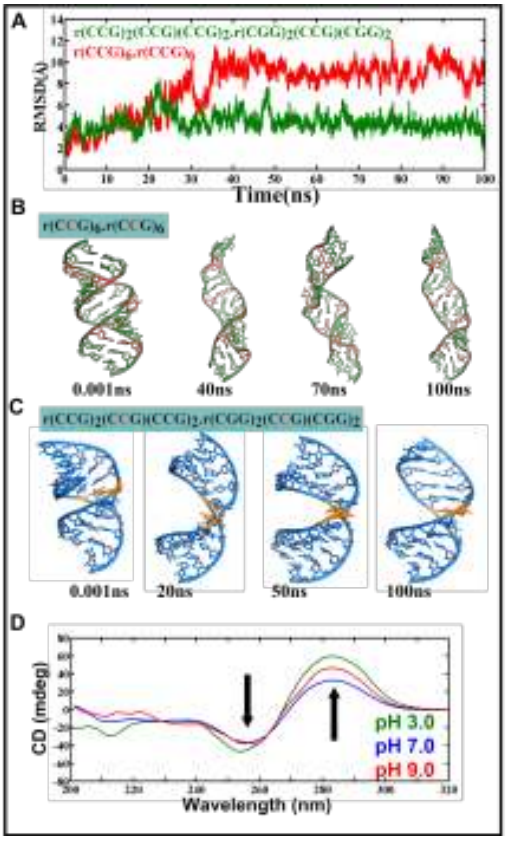


Figure 3.1. Comparison between CCG repeats containing RNA duplexes with one and six C...C mismatches. A) Time vs RMSD profile showing significant conformational changes in RNA duplex with 6 C...C mismatches as indicated by a high RMSD value (red colored) with respect to RNA duplex containing one C...C mismatch (green colored). B) Snapshots showing the distortion in the helix due to 6 C...C mismatches in r(CCG)6.r(CCG)6 duplex in contrast to C) single C...C mismatch. D) pH dependent circular dichroism spectra showing the formation of i-motif structure for r(CCG)6.r(CCG)6 duplex.

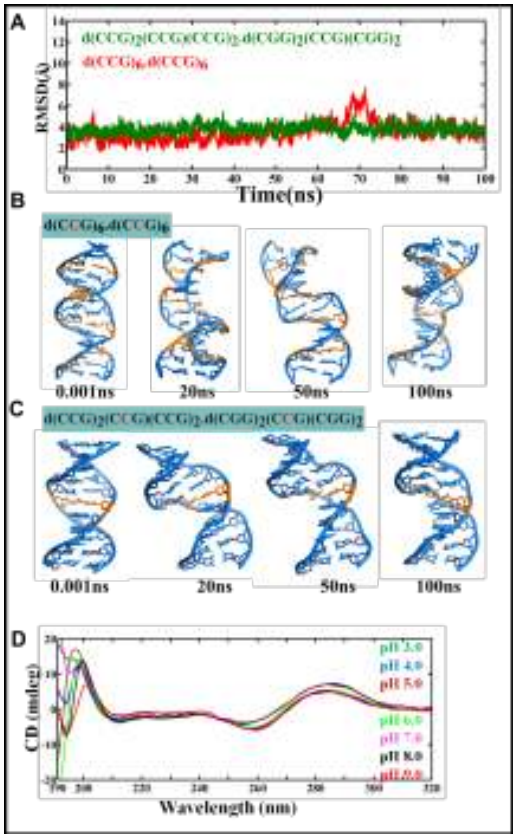
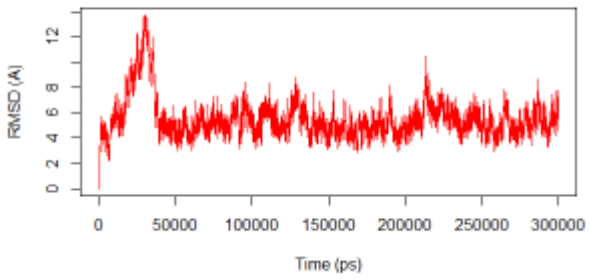


Figure 3.2. Comparison between CCG repeats containing DNA duplexes with one and six C...C mismatches. A) Time vs RMSD profile indicating stable conformation for the DNA duplexes containing one C...C mismatch (green colored) and six C...C mismatches (red colored). B) Snapshots corresponding to DNA containing six C...C mismatches. C) B) Snapshots corresponding to DNA containing one C...C mismatch. D) pH dependent circular dichroism spectra showing the formation of stable DNA duplex for d(CCG)6.d(CCG)6 sequence.

U...U & UC mismatches in CCUG repeats shows A-form geometry.
Expansion of a (CCUG)n tetranucleotide repeat in intron 1 of the cellular nucleic acid binding protein (CNBP) gene on chromosome 3q21 causes a neuromuscular disease called myotonic dystrophy 2(DM2). The characteristics of DM2 are very similar to those observed for DM1 (caused due to CTG repeat expansion in 5 UTR of DMPK gene). Here we studied the secondary structural preference of CC & UC mismatch in CCUG repeats by employing MD simulation technique. Results revealed that overall structure remains stable over 300 ns simulation time.



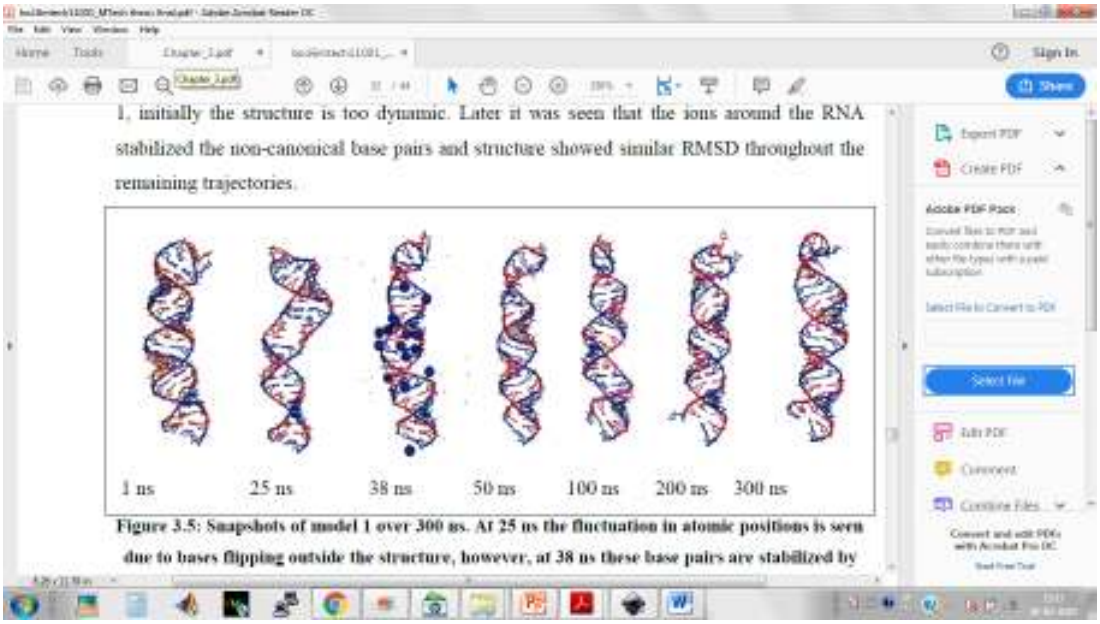


Figure 4. Time vs RMSD profile (top) shows fairly stable structure. Snapshots of model 1 over 300 ns (bottom). At 25 ns the fluctuation in atomic positions is seen due to bases flipping outside the structure, however, at 38 ns these base pairs are stabilized by sodium ions. After that the structure remains fairly stable

Publications / Articles etc. (If any):

Awards (If any):

Dr. K.V.RAO Scientific Society 18th Annual Research Awards 2017-2018, 1st Runner up.

Work presented in conference/s with photographs (if any):

The fifthedition of this Annual Winter Workshop: Computational Biology in DiseaseMechanisms, IITK, December 7-9, 2018, Structural perspectives of trinucleotide repeat expansionsassociated with human diseases: An integrated computational & experimental approach

Appreciation / Recognition (if any):

References:

1. KHAN, N., KOLIMI, N. & RATHINAVELAN, T. 2015. Twisting right to left: A...A mismatch in a CAG trinucleotide repeat overexpansion provokes left-handed Z-DNA conformation. PLoS Comput Biol, 11, e1004162.

2. KOZLOWSKI, P., DE MEZER, M. & KRZYZOSIAK, W. J. 2010a. Trinucleotide repeats in human genome and exome. Nucleic Acids Res, 38, 4027-39.

3. KOZLOWSKI, P., SOBCZAK, K. & KRZYZOSIAK, W. J. 2010b. Trinucleotide repeats: triggers for genomic disorders Genome Med, 2, 29.

4. KRZYZOSIAK, W. J., SOBCZAK, K., WOJCIECHOWSKA, M., FISZER, A., MYKOWSKA, A. & KOZLOWSKI, P. 2012. Triplet repeat RNA structure and its role as pathogenic agent and therapeutic target. Nucleic Acids Res, 40, 11-26

5. LA SPADA, A. R. & TAYLOR, J. P. 2010. Repeat expansion disease: progress and puzzles in disease pathogenesis. Nat Rev Genet, 11, 247-58.

6. MIRKIN, S. M. 2007. Expandable DNA repeats and human disease. Nature, 447, 932-40.

7. USDIN, K. 2008. The biological effects of simple tandem repeats: lessons from the repeat expansion diseases. Genome Res, 18, 1011-9

8. YILDIRIM, I., PARK, H., DISNEY, M. D. & SCHATZ, G. C. 2013. A dynamic structural model of expanded RNA CAG repeats: a refined X-ray structure and computational investigations using molecular dynamics and umbrella sampling simulations. J Am Chem Soc, 135, 3528-38.

Benefits & experience of using NPSF:

To understand the conformational dynamics of biomacromolecules, longer timescale simulation is necessary and NPSF is very much useful in this context. It can be even more beneficial, if queue waiting time can be reduced and more GPU can be inducted.

Any other relevant information (if any): NO

Title of the work carried out: Thermoelectric materials

Name & Designation of the Chief Investigator: V. Kanchana, Professor

E-mail Id: kanchana@iith.ac.in

Institution Name: IIT Hyderabad

Research Challenge/s:

The world we are living is facing several crucial issues such as energy and power crisis and heat wastage, which cause anomalous climate change, ozone layer depletion etc., and the implementation of alternative energy sources which can resolve these issues is very important. Solar energy, wind energy, biomass, tidal energy, hydroelectric, thermoelectricity, etc. are well known alternative energy sources available in nature. Hydroelectric, wind plants are already operating for power generation. The main drawback of these power generation methods are the timely availability of resources, as we know due to the climate changes, water resources are vanishing out. Yet another major issue of our world is heat wastage, survey report says that almost 50% energy is wasting as the form of heat. In this scenario, the importance of solar energy and thermoelectricity are evident. Solar panel and power generation are already in use but localized applications such as in space applications, computer localized applications is challenging with solar energy, where we cannot get the presence of sun light in the spot. Thermoelectric energy conversion stands out among the renewable energy sources for localized applications and waste heat recovery. The challenge in thermoelectric power generation is the lesser efficiency of thermoelectric devices. Several research group have been adequately working for the efficiency improvement. Thermoelectric materials are the materials which can convert waste heat into electricity and the deciding parameter is figure of merit ZT. Our main focus is to understand the thermoelectric properties of different materials and aiming to come up with potential thermoelectric materials. The constituent parameters in ZT is having conflicting dependencies, and getting high value of ZT is highly challenging. Density functional theory is a very prominent tool which successfully predicted several potential thermoelectric materials.

Work carried, Milestone, Achievements & Graphs, Plots:

We have explored several novel thermoelectric materials using our calculations. In this academic year, we have analyzed Os based dichalcogenides, and predicted the same as a potential thermoelectric material with huge thermopower value. We have published our result in Journal of Physics: Condensed matter(JPCM). Further we have analyzed yet another transition metal dichalcogenide ReS2, which is a layered material, and we could show that the bulk, monolayer and bilayer of ReS2 as potential thermoelectric candidate, and published in Journal of solid state chemistry. In addition, we have explored a novel zintl phase series, Ca based compounds, which turned to be potential thermoelectric together with strong topological insulating nature, and we have published the same in Journal of Physics: Condensed matter. A part of all these calculations were performed in CDAC, and we acknowledged the same in all publications.

Publications / Articles etc. (If any):
3 publications have been reported

1. P. C. Sreeparvathy, V. Kanchana, J. Phys. : Conden. Matter, 30, 295501 (2018)

2. PC Sreeparvathy, V Kanchana, P Anees, G Vaitheeswaran, Journal of Solid State Chemistry, 269, 138-144, (2019)

3. P C Sreeparvathy and V Kanchana J. Phys.: Condens. Matter 31 095501 (2019)

Awards (If any): NIL

Work presented in conference/s with photographs (if any):

one invited talk has been delivered and the details are listed below

1. An invited talk on Exploring Novel thermoelectric materials from first principles investigation CMCEE 2018, at Suntec Singapore during 22nd 27th July 2018.

Appreciation / Recognition (if any): –

References: –

Benefits & experience of using NPSF:

Excellent supportive response is obtained from the CDAC help team, and we had several fruitful discussions while compiling all the code which we are using for our calculations. We could get all the information from job submission to the final output, and this system is very helpful. The job status process is very helpful; we could figure out several job terminations without any time delay. Here we sincerely thank the CDAC for this great facility and the good support.

Any other relevant information (if any):

Continued support from the CDAC team is highly appreciated and we look for the same in future with enhanced CPU time as we are working on many other projects also, which might be finished on time with the help of CDAC computing time.

Title of the work carried out: Superconductors

Name & Designation of the Chief Investigator: V. Kanchana, Professor

E-mail Id: kanchana@iith.ac.in

Institution Name: IIT Hyderabad

Research Challenge/s:

A-15 compounds with composition X3Y, where X atoms form three mutually orthogonal chain like structure parallel to the edges of the unit cell, had attracted considerable attention of researcher as some of them possess quite high superconducting transition temperature (Tc).

The interest in these compounds are not only due to the rather high Tc but also their high critical current density and critical magnetic field, along with acceptable mechanical properties make them feasible for applications.

The huge variation of Tc in these compounds are highly challenging and needs a deep insight to understand the same, which forms the main objective of this project In any metal, the shape of the Fermi surface(FS) and wave functions of the electrons at or near the Fermi level are very much useful to explain the properties of the materials. Fermi surface nesting and charge density wave instabilities are reported in this series and they need huge computational resources for computing the same Phonon dispersion of A15 compounds are quite challenging and will be addressed in the present project

Work carried, Milestone, Achievements & Graphs, Plots:

Density functional calculations of few A15 compounds are performed both at ambient and under compression. Mechanical stability is confirmed from the calculated elastic constants both at ambient and under compression in all the compounds. Camel‘s back type band structure features are observed at Fermi level in some of the investigated compounds which causes high density of states at the Fermi level. Fermi surface nesting is observed from the imaginary part of Lindhard susceptibility calculations at ambient. Under compression electronic topological transitions are observed in all the compounds at different compressions.

Publications / Articles etc. (If any):

One manuscript is under preparation P. Rambabu and V. Kanchana, Electronic topological transitions in A-15 type X3Y compounds under compression: A first-principles study

Awards (If any): —-

Work presented in conference/s with photographs (if any): —

Appreciation / Recognition (if any): —

References:—

Benefits & experience of using NPSF:

Excellent supportive response is obtained from the CDAC help team, and we had several fruitful discussions while compiling all the code which we are using for our calculations. We could get all the information from job submission to the final output, and this system is very helpful. The job status process is very helpful; we could figure out several job terminations without any time delay. Here we sincerely thank the CDAC for this great facility and the good support.

Any other relevant information (if any):

Continued support from the CDAC team is highly appreciated and we look for the same in future with enhanced CPU time as we are working on many other projects also, which might be finished on time with the help of CDAC computing time.

Title of the work carried out: First principles study of topological materials

Name & Designation of the Chief Investigator: V. Kanchana, Professor

E-mail Id: kanchana@iith.ac.in

Institution Name: IIT Hyderabad

Research Challenge/s:

Numerous challenges are faced in the area of research in solid state physics. Here, we try to address few of them. We all know that semiconductor physics is a vast area in context of devices and their use and applications. Nowadays, the electronic devices that we are using, run through device called transistor. This device was a revolutionary invention when it was introduced to world but still it poses some challenges like computing speed in computers etc. The cause of this challenge is uncontrollable heat.This is one challenge. The other challenge is to transfer information in storage devices. Generally, the electronic charge acts as degree of freedom. If we can use spin as another degree of freedom, the data can be transferred quickly. The discovery of new class of materials called topological materials overcomes these challenges. There are different class of topological materials like topological insulator, topological semi-metals, Weyl semi-metals and topological metals. Topological insulator is a class of material which is insulator in bulk but possessing conducting gapped states. These states are surface states which preserve time reversal symmetry. This new class of materials has potential applications in spintronics and dissipation less transistor for quantum computers based on the quantum spin hall effect.

Work carried, Milestone, Achievements & Graphs, Plots:

First principles study of Th based compounds are carried both at ambient and under strain in the framework of density functional theory. The elastic and phonon calculations has been done to check the mechanical and dynamical stability of these systems both at ambient and under strain and we found these compounds both mechanically and dynamically stable. We extend our self-consistent calculations to electronic structure. The electronic structure calculations reveal that these systems are semiconductors. Due to band inversion near fermi level and amalgamation of SOC, we extend our electronic structure calculations up to surface states calculations, we found that ThOTe is topological insulator at ambient. We have confirmed it with Z2 calculation through computed parities along TRIM points and surface states calculations. Further, we employed hydrostatic strain on these systems and found these systems are metallic under hydrostatic compressive strain. Next, these compounds are layered structure, so we have done monolayer study. The electronic properties for monolayer show that these systems are metallic. The presence of Dirac points near Fermi level motivated to check topological nature in these monolayer systems. From surface states calculations, we have confirmed that ThOS and ThOSe are topological metals.

Publications / Articles etc. (If any):

One manuscript is under preparation

Awards (If any): —-

Work presented in conference/s with photographs (if any): —

Appreciation / Recognition (if any): —-

References: —-

Benefits & experience of using NPSF:

Excellent supportive response is obtained from the CDAC help team, and we had several fruitful discussions while compiling all the code which we are using for our calculations. We could get all the information from job submission to the final output, and this system is very helpful. The job status process is very helpful; we could figure out several job terminations without any time delay. Here we sincerely thank the CDAC for this great facility and the good support.

Any other relevant information (if any):

Continued support from the CDAC team is highly appreciated and we look for the same in future with enhanced CPU time as we are working on many other projects also, which might be finished on time with the help of CDAC.

Title of the work carried out: Electronic structure and properties of piezoelectric materials

Name & Designation of the Chief Investigator: Dr. Vaishali Shah, Assistant Professor

E-mail Id: vaishali@unipune.ac.in

Institution Name: Interdisciplinary School of Scientific Computing, Savitribai Phule Pune University

Research Challenge:

The lead based piezoelectric composites are widely used in transducers, actuators, sensors, resonators etc. The high piezoelectric constant of the lead based piezoelectric ma- terials makes them suitable for use in devices. However, the toxicity of lead is of concern from its impact on humans and hence there is a need to find alternatives for lead based piezoelectrics. Many piezoelectric devices use pressure as a trigger and that necessi- tates the understanding of the pressure dependent piezoelectric behavior. Pressure can cause a phase transformation of the material enabling the material to change phase with release in pressure and convert the stored energy into electrical energy. A rare earth dopant in the piezoelectric material enables the tuning of the pressure dependent be- havior. A fundamental understanding of the pressure dependent behaviour of the lead based piezoelectric material is crucial to enable the search of lead free materials with a similar behavior. Our research uses first principles total energy calculations based on

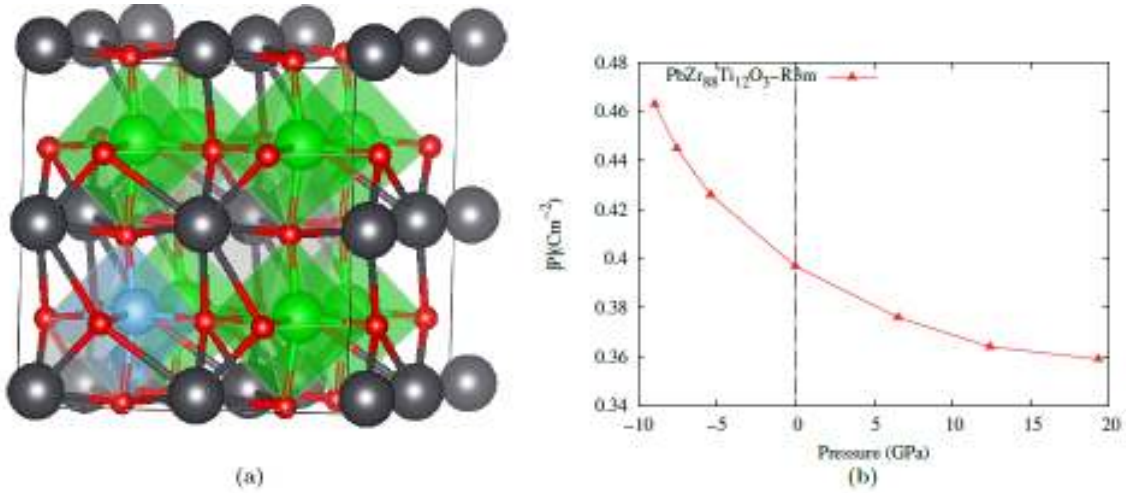


Figure 1: (a) simulation cell of $PbZr_0.88Ti_0.12O_3$ where the corner grey spheres atoms are Pb, red spheres are O, the spheres in the center of the green octahedra are Zr and the sphere in the centre of blue octahedra is Ti; (b) polarization as a function of pressure.

density functional theory and Berry phase simulations to investigate the the piezoelectric behaviour of Lead Zirconium Titanate at di erent compositions.

Work carried :

We are studying the pressure dependent polarization behavior in $PbZr_0.96Ti_0.4O_3$ and

$PbZr_0.88Ti_0.12O_3$ in the ferroelectric and anti-ferroelectric phase. The small percentage of Ti dopant requires the use of large supercells. The theory of polarization and piezoelectric properties are based on density functional perturbation theory and these are extremely computationally expensive. The calculations required to obtain the piezoelectric stress and strain coecients are highly memory intensive and possible only because of access to the high performance capabilities of PARAM YUVA.

Benefits & experience of using NPSF:

Our calculations are highly compute intensive and the access to the NPSF computing resource enabled us to perform these simulations which otherwise were not possible with the available in-house computing resources in our department. Every dif- ficulty with the execution of the jobs submitted on NPSF is promptly addressed by the NPSF help desk and system administrator. Our experience with the NPSF is highly satisfactory and we find them always genial and responsive to our queries and job related issues. NPSF has been a great boon for the research work that is being performed in my research group and I hope that it continues to re- main functional and available to university researchers to take up research problems that cannot be otherwise addressed at our infrastructure level.

Title of the work carried out:ab-initio studies of doped $GaNbO_4$ and TiO_2

Name & Designation of the Chief Investigator: Dr. Vaishali Shah, Assistant Professor

E-mail Id: vaishali@unipune.ac.in

Institution Name: Interdisciplinary School of Scientific Computing, Savitribai Phule Pune University

Research Challenge:

The energy needs of the human race require the development of alternative energy sources to the vanishing hydrofuels. Energy generated from fuel cells and solar cells is of immense interest for being not only renewable but also environmentally clean. There are several challenges that need to me met in this kind of energy generation. The primary being the conversion eciency of the cells and the operability under visible light, the most abundant source of light. The fuel cells have a photocatalytic material to source the hydrogen ions from water that are required for its operation. The photocatalysis of water can be initiated by light absorption that leads to the generation of electron hole pairs and is related with the band gap of the photocatalytic material. The band gaps of the material can be tuned with dopants in order to favor absorption of visible light. With this aim, our study is centered towards the investigation of the absorption behaviour of $GaNbO_4$ which has a band gap similar to the most widely studied photocatalyst TiO_2.

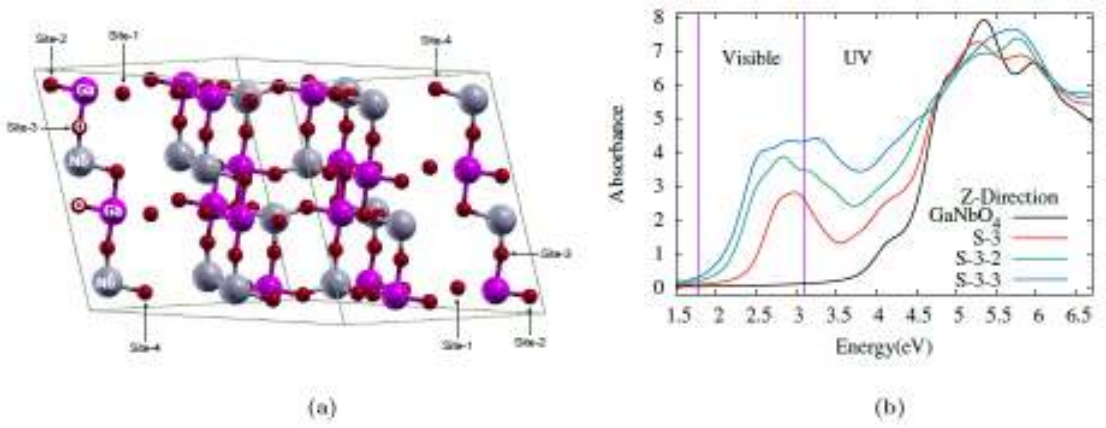


Figure 1: (a) structure of GaNbO4 with the possible dopant sites and (b) absorption spectra of S doped at site-3 with increased concentration of the dopant.

We also investigate the reduction in band gaps due to doping it with S. The research work uses first principles total energy calculations based on density functional theory and are computationally intensive.

Work carried :

Using the PARAM YUVA II high performance computing facility we have been able to study the band structure of pure and doped $GaNbO_4$ and compare it with that of TiO_2. We

have simulated the absorption spectra and are able to understand the absorption behaviour in the visible and UV range of the solar energy spectrum. Our results show that the higher dopant concentration enables a better absorption in the visible range as well as UV range of the solar light energy. The dopant enhances the absorption also in the UV range. We have presented this work at the DAE solid state physics symposium held from December 18-22 2018 and at the National Conference on Advanced Materials Synthesis, Characterization and Applications (AMSCA-2018), held in December 14-15, 2018 at Department of Physics, Savitribai Phule Pune University,Pune.

Benetfis & experience of using NPSF:

Our calculations are highly compute intensive and the access to the NPSF computing resource enabled us to perform these simulations which otherwise were not possible with the computing facilities available in-house at the department. The system administrator of NPSF as well as the help desk has been very supportive and timely in their responses to the difficulties we encountered in the installation of the electronic structure codes as well as the execution of some of the runs because of their memory intensive nature. All the NPSF staff are immensely helpful and cordial and the NPSF computing facility is a life line for the research work in small departments like ours where the resources are very limited. A system like NPSF needs to be maintained and kept running all the time for the benefit of all users and it is a tremendous effort to have it functional throughout the year and this makes us appreciate all the background work of the NPSF team. We certainly hope that more computing resources get added to NPSF and become available through C-DAC for university and college researchers in India.

Title of the work carried out: Novel-Perovskite-SolarCells-PR

Name & Designation of the Chief Investigator: Dr. Yogesh Sonvane

E-mail Id: yas@phy.svnit.ac.in

Institution Name: Sardar Vallbhbhai National Institute of Technology

Research Challenge/s: To find efficiency of perovskite materials

Work carried , Milestone, Achievements & Graphs, Plots:

Publications / Articles etc. (If any):

2D $CH_3NH_3PbI_3$ with High Efficiency and Superior Carrier Mobility: A Theoretical Study (In Press)

Awards (If any): N. A.

Work presented in conference/s with photographs (if any): N. A.

Appreciation / Recognition (if any):

References: N. A.

Benefits & experience of using NPSF: It was good experience to use NPSF facility

Any other relevant information (if any): N. A.

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4.2 Ph.D Theses

1. **Quantifying Uncertainties in Future Climate Change Projections over India**
Scholar: Mr. Ram Singh
Supervisor: Dr. Krishna AchutaRao
Institute: IIT Delhi

2. **First Principles Investigation of Thermally Activated Processes in Pd-based Materials**
Scholar: Mr. Nandha Kumar
Supervisor: Dr. Prasenjit Ghosh
Institute: IISER Pune

3. **Molecular Simulations of Structure and Dynamics of Neat and Hydrated Imidazolium Ionic Liquids**
Scholar: Mr. Praveen Kumar
Supervisor: Dr. Arun Venkatnathan
Institute: IISER Pune

4. **Physical determinant of Gene regulation**
Scholar:Dr. Hungyo Kharerin
Supervisor: Prof. Paike J Bhat
Institute: IIT Bombay

5. **Investigation of Structure, Stability and Strength of intermolecular interactions of some ligandprotein complexes for Alzheimer disease via Molecular docking, Molecular dynamics and QM/MM based charge density analysis**
Scholar: Mr. K. Saravanan
Supervisor: Prof. P. Kumaradhas
Institute: Periyar University

6. **Electronic Structure Transport Properties Using ab initio Calculations: Applications to Low-dimensional Systems**
Scholar: Ms. Deepashri Saraf
Supervisor: Prof. Anjali Kshirsagar,Co-guide: Prof. D. G. Kanhere
Institute: S P Pune University

7. **Wormlike Micelle-Nanoparticle System: A Computational Investigation.**
Scholar: Sk. Mubeena Bano
Supervisor: Dr. Apratim Chatterji
Institute: IISER Pune

8. **Transition Matrix Monte Carlo Methods for the Study of Vapor-Liquid Equilibria of Binary Mixtures**

Scholar: Mr. Tamaghna Chakraborti
Supervisor: Dr. Jhumpa Adhikari
Institute: IIT Bombay

9 **New structural insights into unusual nucleic acid conformation in relevance to mechanisms and pathogeneses of trinucleotide repeat expansion disorders**
Scholar: Mr. Narendar Kolimi
Supervisor: Dr. Thenmalarchelvi Rathinavelan
Institute: IIT Hyderabad

10 **Understanding Photostability of Biomolecules using Multi-reference Quantum Chemical Methods**
Scholar: Mr. Avdhoot Datar
Supervisor: Dr. Anirban Hazra
Institute: IISER Pune

11 **Mechanistic Investigation of Photochemistry and Chemiluminescence using Multi-configurational Quantum Chemistry**
Scholar: Mr. Mahesh Gudem
Supervisor: Dr. Anirban Hazra
Institute: IISER Pune

12 **Electronic Structure Study of Confined Systems**
Scholar: Mr. Prashant Gaikwad
Supervisor: Dr. Anjali K Shirsagar
Institute: S P Pune University

13 **Electronic and Transport Properties of Low Dimensional Materials**
Scholar: Mr. Aniruddha Kibey
Supervisor: Dr. Anjali K Shirsagar
Institute: S P Pune University

14 **Investigation of structural dynamics and allosteric mechanism of SAMHD1 protein complex via Molecular Dynamics studies.**
Scholar: Mr. Kajwal Kumar Patra
Supervisor: Prof. Swati Bhattacharya
Institute: IIT Bombay

15 **Theoretical investigations on interactions among molecules, hydrogen bonded water clusters and their response to externally applied electric fields**
Scholar: Ms. Nalini Dattatraya Gurav
Supervisor: Dr. Rajeev K. Pathak
Institute: S P Pune University

4.3 Publications

Publications by NPSF users

Publications in Peer-Reviewed National and International Journals (with their impact factor)

Following publications resulted from NPSF usage by its users. The publications are listed by the impact factors of the journal they are published in. The impact factor (IF) of an academic journal is a measure reflecting the average number of citations to recent articles published in the journal.

Nano Energy (13.120)

Deepashri Saraf, Sudip Chakraborty, Anjali Kshirsagar, Rajeev Ahuja, "In pursuit of bi-functional catalytic activity in PdS 2 pseudo-monolayer through reaction coordinate mapping" , Nano Energy ,49, 283-289 (2018)

Nano Letters (12.080)

Matukumilli V. D. Prasad and Baidurya Bhattacharya, "Phononic Origins of Friction in Carbon Nanotube Oscillators", Nano Lett. 17, 2131 (2017)

Materials Chemistry A (9.931)

Ashima Rawat, Nityasagar Jena, Dimple, Abir De Sarkar, "A comprehensive study in carrier mobility and artificial photosynthetic properties in Group VI B transition metal dichalcogenide monolayers", Journal of Materials Chemistry A, 6 (2018) 8693-8704

Dimple, Nityasagar Jena, Ashima Rawat, Raihan Ahammed, Manish Kumar Mohanta, Abir De Sarkar*, "Emergence of high piezoelectricity along with robust electron mobility in Janus structures in semiconducting Group IVB dichalcogenide monolayers", Journal of Materials Chemistry A, 6 (2018) 24885-24898

Chemical Sciences (9.063)

SD Yeole, SS Khire, CH Sarode, KD Patil, "On the cationpi interactions in 1, 2-dihydro-1, 2-azaborine",Journal of Chemical Sciences, 2018, Volume 130, Issue 8, Pages103, Publisher Springer India

Acta Crystallographica B (6.467)

Saravanan Manjula, Chinnasamy Kalaiarasi, Mysore S. Pavan, Venkatesha R. Hathwar and Poomani Kumaradhas, "Charge Density and Electrostatic Potential of Anti-Hepatitis C Viral Agent Andrographolide: An Experimental and Theoretical Study", , Acta Cryst Section

B74, 693-704, (2018)

Carbon (6.337)

S Chandra Shekar, R. S. Swathi, "Molecular switching on graphyne and graphdiyne: Realizing functional carbon networks in synergy with graphene", Carbon 2018, 126, 489-499

ACS Omega (5.547)

Tamaghna Chakraborti , Anish Desouza, Jhumpa Adhikari, "Prediction of Thermodynamic Properties of Levulinic Acid via Molecular Simulation Techniques", ACS Omega, 2018, 3 (12), pp 1887718884,DOI: 10.1021/acsomega.8b02793 (2018)

ApJ (5.333)

Korsos, M., Chatterjee, P. and Erdelyi, R, Applying the weighted horizontal magnetic gradient method to a simulated flaring Active Region, 2018, DOI: 10.3847/1538-4357/aab891

Monthly Notices of the Royal Astronomical Society (5.194)

Sharanya Sur (IIA), Pallavi Bhat (MIT) , Kandaswamy Subramanian (IUCAA),"Faraday rotation signatures of fluctuation dynamos in young galaxies", Vol. 475 (2018)

Catalysis Today (4.667)

L. George, S. Sappati, P. Ghosh, R. Nandini Devi, "Sensitizing with short conjugated molecules: Multimodal anchoring on ZnO nanoparticles for enhanced electron transfer characteristics, stability and H2 evolution", Catalysis Today, 309, 89 (2018).

Physical Chemistry C (4.484)

Rejaul Sk, Srilatha Arra, Barun Dhara, Joel S Miller, Mukul Kabir, Aparna Deshpande, "Enhancing the Intermolecular Interaction by Cyano Substitution in CuPc" , J. Phys. Chem. C , 122, 429 (2018)

Sandip R. Kumavat, Yogesh Sonvane , Deobrat Singh, and Sanjeev K. Gupta ,Two-Dimensional CH3NH3PbI3 with High Efficiency and Superior Carrier Mobility: A Theoretical Study, J. Phys. Chem. C, 2019, 123 (9), pp 52315239, DOI: 10.1021/acs.jpcc.8b11427

Srilatha Arra, K. R. Ramya, Rohit Babar and Mukul Kabir, "Photocatalytic Activity of Phosphorene Derivatives: Coverage, Electronic, Optical and Excitonic properties", The Journal of Physical Chemistry C 122, 7194 (2018), DOI:10.1021/acs.jpcc.7b12649

Prasad Rama, Arup R. Bhattacharyya, Rajdip Bandyopadhyaya, Ajay S. Panwar, "Ion Valence and Concentration Effects on the Interaction between Polystyrene Sulfonate-modified Carbon Nanotubes in Water", J. Phys. Chem. C, 2018, 122, 96199631

Rejaul Sk, Srilatha Arra, Barun Dhara, Joel S Miller, Mukul Kabir, Aparna Deshpande , "Effect of Cyano Substitution on the Step-Edge Adsorption of Copper Phthalocyanine on Au (111) ", The Journal of Physical Chemistry C 122, 11848 (2018), DOI:10.1021/acs.jpcc.8b02178

N Kumar, D. Chattaraj, P. Ghosh, and C. Majumder, "Microscopic Insights of Hydrogen Permeation through a Model PdCu Membrane from First Principles Investigations", J. Phys. Chem. C, 122, 12920 (2018).

V. Kumar, N. Joshi, B. Dhara, P. Jha, S. Rana, P. Ghosh, N. Ballav , "Stable Red Emission from Nanosheets of Molecularly Doped Hexagonal Boron Nitride", J. Phys. Chem. C, 122, 21076 (2018).

J. Mol. Biol (4.333)

H. Maity and G. Reddy, Thermodynamics and kinetics of single chain Monellin folding with structural insights into specific collapse in the denatured state ensemble, J. Mol. Biol., 2018 Feb 16;430(4):465-478 DOI: 10.1016/j.jmb.2017.09.009, 2017

International Journal of Biological Macromolecules (3.909)

Penislusshiyan, Sakayanathan, Chitra Loganathan, Ancy Iruthayaraj, Premkumar Periyasamy, Kumaradhas Poomani, Viswanathamurthi Periasamy, Palvannan Thayumanavan, "Biological interaction of newly synthesized astaxanthin-s-allyl cysteine biconjugate with Saccharomyces cerevisiae and mammalian α-glucosidase: In vitro kinetics and in silico docking analysis", International Journal of Biological Macromolecules, 118, 252-262, 2018

Physical Chemistry Chemical Physics (3.906)

A. Gahlaut and M. Paranjothy, "Unimolecular decomposition of formamide via direct chemical dynamics simulations", Physical Chemistry Chemical Physics, 20, 8498 - 8505 (2018)

Physical Review B (3.836)

V. R. Chandra and J. Sahoo, "Spin- 1 2 Heisenberg antiferromagnet on the pyrochlore lattice: An exact diagonalization study",Phys. Rev. B 97, 144407 (2018)

Rohit Babar, Mukul Kabir , "Gate-dependent vacancy diffusion in graphene",Physical Review B 98, 075439 (2018), DOI: 10.1103/PhysRevB.98.075439

Rohit Babar and Mukul Kabir,"Engineering Kondo state in two-dimensional semiconducting phosphorene", Physical Review B 97, 045132 (2018), DOI:10.1103/PhysRevB.97.045132

Soft Matter (3.709)

P. Kumar, P. Prakash, K. R. Ramya and A. Venkatnathan, "Probing Translational and Rotational Dynamics in Hydrophilic/Hydrophobic Anions based Imidazolium Ionic Liquid-water mixtures", Soft Matter, 14, 6109 (2018).

Atmospheric Environment (3.70)

Sumita Kedia, R Kumar, S Islam, Y Sathe, A Kaginalkar, "Radiative impact of a heavy dust storm over India and surrounding oceanic regions", Atmospheric Environment, 185, 109-120 (2018)

Polymer (3.483)

Rajesh Kumar, Avinash Parashar, "Effect of geometrical defects and functionalization on the interfacial strength of h-BN / polyethylene based nanocomposite",Polymer, (2018), 146, 82-90.

Nanotechnology (3.404)

Sivasubramani, S., Debroy, S., Acharyya, S. G. & Acharyya, "A. Tunable intrinsic magnetic phase transition in pristine single-layer graphene nanoribbons", Nanotechnology 29, 455701, doi:10.1088/1361-6528/aadcd8 (2018).

Biochimie (3.188)

Johnson Preethi, Loganathan Chitra, Iruthayaraj Ancy, Poomani Kumaradhas, Thayumanavan Palvannan , "S-allyl cysteine as potent anti-gout drug: Insight into the xanthine oxidase inhibition and anti-inflammatory activity", Biochimie, 154, 1-9 , (2018)

Physical Chemistry B (3.146)

Bappa Ghosh and Srabanti Chaudhury, "Influence of the Location of Attractive Polymer Pore Interactions on Translocation Dynamics", J. Phys. Chem. B, 122,360-368 (2018)

Sangkha Borah, P. Padma Kumar, "First Principle Molecular Dynamics Investigation of Waterborne As-V Species"(accepted)2018

Industrial & Engineering Chemistry Research (3.141)

Tamaghna Chakraborti , Jhumpa Adhikari ,"VaporLiquid Equilibria of Mixtures of Molec-

ular Fluids Using the Activity Fraction Expanded Ensemble Simulation Method", Ind. Eng. Chem. Res., 2018, 57 (36), pp 1223512248,DOI: 10.1021/acs.iecr.8b02067 (2018)

Biomolecular Structure and Dynamics (3.107)

Rajneet Kaur Sani, Suniba Shuaib, Deepti Goyal, Bhupesh Goyal, "Insights into the Inhibitory Mechanism of a Resveratrol and Clioquinol Hybrid against Aβ42 Aggregation and Protofibril Destabilization: A Molecular Dynamics Simulation Study", J. Biomol. Struct. Dyn, 1. (2018)

Chinnasamy Kalaiarasi, Saravanan Manjula and Poomani Kumaradhas, "Evaluation of binding and antagonism/downregulation of Brilanestrant molecule in Estrogen receptor-α via Quantum mechanics/Molecular mechanics", Molecular dynamics and Binding free energy calculations, Journal Biomolecular Structure and Dynamics, 2018.

Magudeeswaran Sivanandam, Saravanan Manjula & Poomani Kumaradhas, "Investigation of activation mechanism and conformational stability of N-(4-chloro-3-trifluoromethyl-phenyl)-2-ethoxybenzamide and N-(4-chloro-3-trifluoromethyl-phenyl)-2-ethoxy-6-pentadecyl-benzamidein the active site of p300 histone acetyl transferase enzyme by molecular dynamics and binding free-energy studies", Journal Biomolecular Structure and Dynamics, (2018), https://doi.org/10.1080/07391102.2018.1533497

Saravanan, K., Sivanandam, M., Hunday, G., Mathiyalagan, L., Kumaradhas, "Investigation of Intermolecular interactions and Stability of Verubecestat in the active site of BACE1: Development of First model from QM/MM based Charge density and MD Analysis", P, Journal Biomolecular Structure and Dynamics, (2018), https://doi.org/10.1080/07391102.2018.1479661

Saravanan Manjula, Magudeeswaran Sivanandam, Poomani Kumaradhas, "Probing the fingers domain binding pocket of Hepatitis C virus NS5B RdRp and D559G resistance mutation via Molecular Docking, Molecular Dynamics simulation and binding free energy calculations", Journal of Biomolecular Structure and Dynamics, (2018), DOI: 10.1080/07391102.2018.1491419

M. Sivanandam, K. Saravanan, P. Kumaradhas, "Insights into Intermolecular interactions, electrostatic properties and the stability of C646 in the binding pocket of p300 Histone acetyltransferase enzyme: A combined molecular dynamics and charge density study", Journal of Biomolecular Structure and Dynamics, (2018) 36 (12), 3246-3264.

Materials Science (2.993)

V. Kumar and D. R. Roy, Structure, Bonding, Stability, Electronic, "Thermodynamic and Thermoelectric Properties of Six Different Phases of Indium Nitride", J. Mat. Sci. (Springer Link) 53 (2018) 8302-8313.

Cellular Biochemistry (2.959)

Rajneet Kaur Sani, Suniba Shuaib, Deepti Goyal, Bhupesh Goyal, "Molecular Insights into the Effect L17A/F19A Double Mutation on the Structure and Dynamics of Aβ40: A Molecular Dynamics Simulation Study", J. Cell. Biochem. 2018, 119, 8949

Simranjeet Singh, Narang, Suniba Shuaib, Deepti Goyal, Bhupesh Goyal, "Assessing the Effect of D59P Mutation in the DE Loop Region in Amyloid Aggregation Propensity of β2-Microglobulin: A Molecular Dynamics Simulation Study", J. Cell. Biochem, 119, 782 (2018)

Saini, R. K.; Shuaib, S.; Goyal, D.,Goyal, B., "Molecular insights into the effect L17A/F19A double mutation on the structure and dynamics of Aβ40: A molecular dynamics simulation study", J. Cell. Biochem. 2018, 119, 8949

Applied Nanoscience (2.951)

K. Rajput, D. R. Roy," h-CaS and h-CaSe nanosheets in CaX (X = O, S, Se and Te) series: promising thermoelectric materials under DFT investigation", DOI: 10.1007/s13204-019-00997-4

Physical Review A (2.925)

N. M. Fazil, V. S. Prasannaa, K. V. P. Latha, M. Abe, and B. P. Das, Phys. Rev. A 98, 032511 (2018) "LZ15977AR - RaH as a potential candidate for electron electric dipole moment searches".

IEEE Transactions on Nanotechnology (2.857)

Boddepalli SanthiBhushan, Mohammad Shahzad Khan, Vijay Kumar Bohat, and Anurag Srivastava, "Quantum Capacitance Estimations of Pyrrolic-Rich Graphene for Supercapacitor Electrodes", IEEE Transactions on Nanotechnology 17, no. 2 (2018): 205-211.

Physical Chemistry A (2.836)

Mahesh Gudem and Anirban Hazra, "Intersystem Crossing Drives Photoisomerization in o-Nitrotoluene, a Model for Photolabile Caged Compounds", J. Phys. Chem. A, (2018), 122, 48454853

E. G. Naz, S. Godara, M. Paranjothy, "Direct chemical dynamics simulations of H3+ + CO bimolecular reaction", J. Phys. Chem. A, 122, 8497 - 8504 (2018)

Environmental Toxicology and Pharmacology (2.776)

Thayumanavan Palvannan, Loganathan Chitra, Iruthayaraj Ancy, Poomani Kumaradhas,

Nallaiyan Selvan , "S-allyl-glutathione, a synthetic analogue of glutathione protected liver against carbon tetrachloride toxicity: Focus towards anti-oxidative efficiency", Environmental Toxicology and Pharmacology, 58, , 21-28. (2018)

Physics: Condensed Matter (2.617)

P. C. Sreeparvathy, V. Kanchana, "Giant thermopower in 'p' type OsX2 (X: S, Se, Te) for a wide temperature range: a first principles study",J. Phys.: Conden. Matter, 30, 295501 (2018)

Mohammad Aslam, Chandan Singh, Shekhar Das, Ritesh Kumar, Soumya Datta, Soumyadip Halder, Sirshendu Gayen, Mukul Kabir, Goutam Sheet, "Large enhancement of superconductivity in Zr point contacts",Journal of Physics: Condensed Matter 30, 255002 (2018) [DOI:10.1088/1361-648X/aac154]

Fluid Phase Equilibria (2.197)

Tamaghna Chakraborti, Jhumpa Adhikari, "Study of fluid phase equilibria of triangle-well mixtures in bulk and under confinement using grand canonical transition matrix Monte Carlo Author links open overlay panel", Fluid Phase Equilibria Volume 478 (2018) Pages 42-57

Applied Physics (2.176)

Bhavna C. Keswani, Deepashri Saraf, S. I. Patil, Anjali Kshirsagar, A. R. James, Y. D. Kolekar, and C. V. Ramana, "Role of A-site Ca and B-site Zr substitution in BaTiO3 lead-free compounds: Combined experimental and first principles density functional theoretical studies" , Journal of Applied Physics, 123, 204104 (2018)

Molecular Structure (2.011)

Chinnasamy Kalaiarasi, Pachamuthu Sangeetha, Mysore S. Pavan, Poomani Kumaradhas, "Crystal structure and theoretical charge density studies of dilantin molecule", Journal of Molecular Structure 1170 105-118, (2018)

Molecular Graphics and Modelling (1.885)

N.S. Venkataramanan, A. Suvitha, Nature of bonding and cooperativity in linear DMSO clusters: A DFT, AIM and NCI analysis "Journal of Molecular Graphics and Modelling 81 (2018) 50-59."

International Journal of Mass Spectrometry (1.826)

Y. Krishnan, P. Rajbangshi, and M. Paranjothy, "Theoretical study of perbenzoate anion decomposition pathways in the gas phase", International Journal of Mass Spectrometry, 428, 8 14 (2018)

Geophysical & Astrophysical Fluid Dynamics (1.417)

Chatterjee, "Testing Alfven wave propagation in a realistic set-up of the solar atmosphere", P (2018), GAFD (arXiv:1806.08166)

Meteorology and Atmospheric Physics (1.36)

Sumita Kedia, R Vellore, S. Islam, A Kaginalkar, "A study of Himalayan extreme rainfall events using WRFChem", Meteorology and Atmospheric Physics, 1-11 (2018)

Theoretical and Computational Fluid Dynamics (1.23)

Sethuraman, Y. P. M., Sinha, K., Larsson, J., "Thermodynamic fluctuations in canonical shock-turbulence interaction: effect of shock strength.", Theoretical and Computational Fluid Dynamics, Vol. 32, Issue 5, pp. 629654 (2018)

Astronomische Nachrichten (0.916)

Brandenburg A. and Chatterjee, P, Strong nonlocality variations in a spherical mean-field dynamo, Astron. Nachr. 339, 118-126 (2018), DOI: 10.1002/asna.201813472

Conferences 2018:

ASCE India Conference 2017

M. C. Raghucharan , Surendra Nadh Somala, Generating Site-Specific Ground Motions for Delhi Region for Seismic Vulnerability Assessment of BuildingsPromoting Disaster Resilient Communities

16th Symposium on Earthquake Engineering

M. C. Raghucharan , Surendra Nadh Somala, Venkata Kishor Gangapogu, "Synthetic Ground Motions for Mw 6.5 Hypothetical Earthquake and Comparison of Structural Response with Combination Rules of IS 1893-Part 1 (2016)"

63rd DAE SSPS

Mohammad Ubaid, BS Pujari, A Aziz, "First principle study of In/Ga/doped Phosphorene", 63rd DAE SSPS (2018), Center for Modelling and Simulation, SP Pune University held at GJUST Hisar organized by 63rd DAE SSPS, 18-22 December 2018.

International Conference on Advanced Computing (ICoAC) Conference

Vinaya Sivanandan, Amol Wagare, Vikas Kumar, "Development of 3D Navier-Stokes Solver for CFD on GPU", International Conference on Advanced Computing (ICoAC) Conference, Anna University, Chennai, (2018)

FMFP2018

Popat Bangar, Siddharth Jabade, Chetan Khare, Vikas Kumar, Gaurav Marskole, Kedar Sant, Manisha Mhetre, Mangesh Chaudhari , Development of Sensor for Measurement of Various Parameters in Data Centre, FMFP2018PAPER NO.611.

Paper: Submitted (under review)

Sharanya Sur (IIA), "Decaying turbulence and magnetic fields in galaxy clusters" MNRAS (submitted)

G. Sharma, S. Datta, P. Ghosh, "First Principles Study of Thermoelectric Properties of Bulk and a Monolayer of Bismuth Iodide", ACS Omega. (Submitted)

Aswathi Mohan T and P Ghosh, "Antiferromagnetic semiconducting 1T to ferromagnetic halfmetallic 1H phase transition in Ti2C MXenes: A Theoretical Prediction", Phys. Rev. B (submitted)

N. Joshi, C. Gaurav, N. Ballav, and P. Ghosh, "O intercalation induced enhancement of magnetic moments and surface reconstruction at graphone/Ni (111) interface: A first principles prediction", Phys. Rev. B.(submitted)

Sumita Kedia, S K Das, S Islam, A.Hazra, N. Kumar, "Aerosols impact on the convective and non-convective rain distribution over the Indian region: Results from WRF-Chem simulation", Atmospheric Environment, Accepted (2018)

K. Mondal and P. Ghosh, "Exfoliation of Ti2C and Ti3C2 MXenes from bulk phases of Titanium Carbide: A theoretical prediction", Comp. Mat. Sc. (submitted)

N. Kumar, D. Chattaraj, I. Kaul, C. Majumdar, P. Ghosh, "First-principles investigation of growth of small Pd-Ga bimetallic clusters on MgO(100) surface",J. App. Phys.(submitted)

V. Kumar and D. R. Roy, "Structure, Electronic, Vibrational Properties of Single-Layer Stanane and its Application as a Potential Gas Sensor for NO2, SO2, CO2 and NH3", Phys. Chem. Chem. Phys. (Royal Soc. Chem.) (2018)

Kajwal Kumar Patra, Akash Bhattacharya and Swati Bhattacharya, "Molecular dynamics investigation of a redox switch in the anti-HIV protein SAMHD1" (under review)

Ankush Bharti, Neha Katoch, Raman Sharma and P K Ahluwalia, Stability, Electronic and Optical Properties of In-Plane WSe2 Heterophase Nano-ribbons, (submitted)

5

Visits

Total number of visitors during Year-2018 : 2178

5.1 Visits by Dignitaries

- Prof. D. N. Reddy, Director, CR Rao AIMSCS, HCU, Hyderabad.
- Dr. Ajay K. Nayak, Joint Secretary, Govt of Odisha, Bhubaneswar.
- Prof. R. K. Singh, Dean (Students Welfare), MNNIT, Allahabad.
- Shri. M. Krishna, Assistant Director (DOC), Central Forensic Science Laboratory (CFSL), Hyderabad.
- Wing Commander A. Ahluwalia, Indian Air Force.
- Dr. Bahgat Sammakia, Interim President, SUNY Polytechnic Institute, New York.
- Shri. Jual Oram, Honble Minister of tribal affairs, Govt of India.
- Wing Commander M.M. Ingale, Indian Air Force
- Makarand Kedare, Deputy General Manager, IT Innovations,State Bank of India.
- Israr Sheikh and Narasimha Ranganathan
- Judges of the High Court of Bombay, Madhya Pradesh, Punjab, Haryana and Delhi.
- Ashok Chakradhar, Former professor and head of the department of Hindi atJamia Millia Islamia
- Vivek M Hirpathak, Chief Operating Officer at Indra Networks, , Pune
- Ms.Anuradha Mitra, AS&FA,MeitY, New Delhi.
- ShriRajiv Kumar,Joint Secretary, MeitY, New Delhi
- Shri SanjayGoel, Joint Secretary, MeitY, New Delhi
- Prof. Dhiren Patel, Pro-Vice Chancellor, University ofMumbai.
- Prof. Vladimir Voevodin, Deputy Director for Research, Research Computing Center, Lomonosov Moscow State University

- Mr. Azevedo , LNCC, Director , Brazil.
- Philippe O. A. Navaux, Professor Informatics Institute GPPD/INF/UFRGS, Brazil
- inga Reddy, Assistant Commissioner, Election Commission, Banglore.
- JeffreyCBuchsbaum, Medical Officer and Program Director,National Cancer Institute, Bethesda, USA.
- Ramesh Loganathan,Professor of Practice, Co-innovations, IIT Hyderabad
- Mr. Deepak Prasad, SSE(SIM), SDI, AF
- R Jagadeesh Kannan. Professor, School of Computing Science and Engineering,VIT University, Chennai.
- Dr. N. Sambandam , Pro-Vice Chancellor, VIT University, Chennai
- Ryan Laemel,Manager, Rocky Mountain Institute, Basalt, USA.
- ShriGopalakrishnan S., Joint Secretary, MeitY, New Delhi
- Shri S. K. Arora, Dy. Director, IFD, Meity, New Delhi.
- Khurshid Sultan, Director of JNIUCII,Uzbekistan
- Col (Retd) Arun Kumar, Executive Editor in DEFPROAC ,Col SI-2(C), ADGSI DTE, IDS
- Shri. Sunil Barthwal, IAS CPFC, EPFO and Additional Secretary of Govt. of India.
- Dr. P. K. Khosala, Executive Director, Mohali.
- Venkatesh Raghavan,Professorof Geoinformatics,Osaka City University
- Mr.Vinay Thakur,Director, National E-Governance Division (NEGD),Meity.
- Dr.T.P. Singh.Director, Bhaskaracharya Institute of Space Application and. Geo-informatics, Gujrat.
- Dr. K. S. Rajan, Associate Professor, International Institute of Information Technology, Hyderbad.
- Mr.Suhas Punekar, Managing Director Punekar Educational Initiaves,Washim, Maharashtra.

5.2 Visits by Academic Institutions

Table 5.1: Summary of Industrial Visits

Institution	No. of visitors
2018	
AISSMS COE, Shivajinagar, Pune	50
G H Raisoni College of Engg	30
Royal College of Science, Mira Road	50
Latthe Edn Soc, Sangli	41
Dr Manoj Shette College of engineering Kasara	25
Knowledge Institute of Technology and Engineering	40
Govt. Engineering College, Bikaner	50
Matoshri College, Mumbai	60
Marwadi Education Foundation, Rajkot	50
Thakur Education, Mumbai	120
LNCT Campus, Bhopal	60
Neotech Institute of Technology ,Vadodara	60
St.Jhon College of Engineering, Palghar	50
Gujarat Technological University, Ahmedabad	23
Symbiosis International University,Pune	22
JSPM's Imperial College of Engineering & Research, Wagholi	40
Siddhant College of Enggineering, Sudumbare	50
Pune Institute of Computer Technology	120
Trinity Polytechnic, Pune	25
Pimpri Chinchwad Polytechnic	70
AISSMS COE, Pune	50
St. Mira's college, Pune	30
Marwadi Education Foundation, Rajkot	50
AISSMS Polytechnic, Pune	80
Gharda Institute of Technology (GIT), Lavale	45
Vidyalankar Polytechnic, Wadala	50
Government Polytechnic, Karad	72
RBS Engg. Tech. Campus, Bichpuri, Agra	60
AISSMSIOIT, PUNE	50
Sardar Patel College, Anand	40
Theem College	50
Bhivarabai Sawant College of Engg. & Research, Pune	60
St. Francis Institute of Technology(SFIT)	90
Modern College Of Engineering	50

Continued on next page

Table 5.1 – *Continued from previous page*

Institution	**No. of visitors**
COEP, Pune	20
P.C. JABIN SCIENCE COLLEGE, Vidhyanagar, Hubballi	50
MIT-WPU, Karad	180
Regal College of Techology, Chiplun	25
Gurukul Polytechnic, Nandgaon (Nashik)	45
Total	2178

Appendices

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Appendix A

Users across Institutions

Below is the list of NPSF users across Institutions

Table A.1: Users across Academic Institutions

State	Academic Institutions	No. of Users
Assam	Assam University, Silchar	1
	Dibrugarh University, Dibrugarh	3
	Indian Institute of Technology (IIT), Guwahati	22
	National Institute of Technology (NIT), Silchar	2
Bihar	Central University of South Bihar (CUSB), Patna	1
	Indian Institute of Technology (IIT), Patna	8
Chandigarh	Panjab University , Chandigarh	6
Delhi	Guru Gobind Singh Indraprastha University, Delhi	3
	Indian Institute of Technology (IIT), Delhi	8
	Indraprastha Institute of information technology, Delhi	4
	Jamia Millia Islamia University, New Delhi	5
	Jawaharlal Nehru University (JNU), Delhi	2
	University of Delhi, New Delhi	4
Goa	Goa University	2
Gujarat	Central University of Gujarat (CUG), Gandhinagar	3
	Gujarat Technological University (GTU), Ahmedabad	1
	Indian Institute of Technology (IIT), Gandhi Nagar	10
	Sardar Vallabhbhai National Institute of Technology (SVNIT) , Surat	11
	St. Xaviers College, Ahmedabad	1
Haryana	Central University of Haryana (CUH), Jant-Pali	3
	Kurukshetra University, Kurukshetra	3

Continued on next page

Table A.1 – *Continued from previous page*

State	Academic Institutions	No. of Users
Himachal Pradesh	Central University of Himchal Pradesh (CUHIMACHAL), Shahpur	2
	Himachal Pradesh University , Shimla	7
Jharkhand	Indian Institute of Technology (Indian school of Mines) (IITISM) , Dhanbad	3
Karnataka	Indian Institute of Astrophysics, Bengaluru	12
	Indian Institute of Science (IISC), Bengaluru	7
	LGC Promochem India Pvt Ltd, Bengaluru	1
	Manipal University, Bengaluru	2
	University of Mysore, Mysuru	2
Kerala	Indian Institute of Science Education and Research (IISER), Thiruvananthapuram	3
	National Institute of Technology (NIT), Calicut	1
Madhya Pradesh	ABV - Indian Institute of Information Technology and Management (ABV- IIITM), Gwalior	6
	Jiwaji University, Gwalior	3
Maharashtra	Ahmednagar College, Ahmednagar	1
	Army Institute of Technology(AIT), Pune	5
	Bhusawal Arts, Science and PO Nahata CommerceCollege, Jalgaon	1
	College of Engineering (COEP), Pune	6
	D Y Patil University, Pune	3
	H.P.T Arts and R.Y.K. Science College, Nasik	1
	Indian Institute of Science Education and Research (IISER), Pune	61
	Indian Institute of Technology (IIT), Bombay	248
	JSPM TSSM College, Pune	1
	Maharashtra Institute of Technology, Pune	1
	Padmabhooshan Vasantdada Patil Institute of Technology (PVPIT), Pune	3
	Rashtrasant Tukadoji Maharaj Nagpur University (RTMNU), Nagpur	2
	Savitribai Phule Pune University, Pune	39
	Swami Ramanand Teerth Marathwada University (SRTMUN), Nanded	2
	Symbiosis Institute of Technology (SIT), Pune	1
	Tetrahydrix Engg. Pvt. Ltd. (TEPL), Pune	1
	Visvesvaraya National Institute of Technology (VNIT), Nagpur	10
	Whistling Woods International Institute (WWII), Mumbai	2
Mizoram	Pachhunga University College , Aizawl	1

Continued on next page

Table A.1 – *Continued from previous page*

State	Academic Institutions	No. of Users
Odisha	Indian Institute of Technology (IIT), Bhubaneswar	4
	National Institute of Technology Rourkela (nitrkl)	1
Pondicherry	Pondicherry University, Pondicherry	5
Punjab	Guru Nanak Dev University, Amritsar	1
	Indian Institute of Science Education and Research (IISER), Mohali	1
	Indian Institute of Technology (IIT), Ropar	8
	Institute of Nano Science and Technology (INST), Mohali	23
	Sri Guru Granth Sahib World University, Fatehgarh Sahib	9
Rajasthan	Cetral University of Rajsthan (CURAJ), Ajmer	1
	Government College, Tonk	1
	Indian Institute of Technology (IIT), Jodhpur	12
	Pandit Deendayal Upadhyaya Shekhawati University, Sikar	1
	University of Rajastan, Jaipur	1
Tamil Nadu	Anna University, Chennai	2
	Shanmugha Arts, Science, Technology & Research Academy (SASTRA), Thanjavur	3
	University of Madras, Chennai	1
	SRM Institute of Science and Technology, Kattankulathur	3
Telangana	BITS Pilani, Hyderabad	2
	CMR College of Engineering & Technology (CMRCET), Hyderabad	2
	GITAM university, Hyderabad	1
	Indian Institute of Technology (IIT), Hyderabad	34
	International Institute of Information Technology (IIIT), Hyderabad	4
	Osmania University, Hyderabad	2
	Professor Jayashankar Telangana State Agricultural University(PJTSAU), Hyderabad	1
	University of Hyderabad, Hyderabad	1
Uttar Pradesh	Aligarh Muslim University (AMU), Aligarh	5
	Amity University, Noida	2
	GLA University, Mathura	1
	Indian Institute of Technology (IIT), Kanpur	25
Uttarakhand	Indian Institute of Technology (IIT), Roorkee	5

Continued on next page

Table A.1 – *Continued from previous page*

State	Academic Institutions	No. of Users
West Bengal	Indian Institute of Science Education and Research (IISER), Kolkata	2
	Indian Institute of Technology (IIT), Kharagpur	13
	Total	**718**

Table A.2: Users across research institutions

State	Research Institutions	No. of Users
Assam	Institute of Advanced Study in Science and Technology (IASST), Guwahati	4
Delhi	National Informatics Centre, Delhi	2
Gujarat	Indian Space Research Organisation (ISRO), Ahmedabad	5
	Physical Research Laboratory (RRL), Ahmedabad	3
Haryana	Dr.Vijay Kumar Foundation, Gurgaon	9
	Translational Health Science and Technology Institute (THSTI) , Faridabad	4
Karnataka	GARUDA	165
	Indian Air Force (INAF), Bengaluru	1
	Indo-Korea Science and Technology Centre (IKST), Bengaluru	1
	Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), Bengaluru	11
	Raman Research Institute (RRI), Bengaluru	3
Madhya Pradesh	UGC DAE Consortium for Scientific Research, Indore	1
Maharashtra	Bhabha Atomic Research Centre (BARC), Mumbai	1
	Centre for Development of Advanced Computing (CDAC)	151
	CSIR-National Chemical Laboratory (CSIR-NCL), Pune	9
	E-teacher	2
	Inter-University Centre for Astronomy and Astrophysics (IUCAA), Pune	7
	National Centre for Radio Astrophysics(NCRA), Pune	6
	The Institute of Science, Mumbai	2
	UM-DAE Centre for Excellence in Basic Sciences, Mumbai	3
Manipur	Institute of Bioresources and Sustainable Development (IBSD), Imphal	2

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Table A.2 – *Continued from previous page*

State	Research Institutions	No. of Users
Odisha	National Institute of Science Education and Research (NISER), Bhubaneswar	2
Punjab	National Agri-Food Biotechnology Institution (NABI), Mohali	1
Tamil Nadu	Central ElectroChemical Research Institute (CSIR), Karaikudi	4
	DRDO-BU Centre for life Sciences, Coimbatore	4
Uttar Pradesh	Bharat Petroleum Corporate Research and Development Centre, Noida	2
	Harish-Chandra Research Institute(HRI), Allahabad	2
West Bengal	Central Inland Fisheries Research Institute (CIFRI),Kolkata	2
	Indian Association for the Cultivation of Science(IACS), Kolkata	1
	Saha Institute of Nuclear Physics, Kolkata	2
	Total	**412**

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Appendix B

Projects Enrolled during Year 2018

The list of projects from various institutions using NPSF compute time with the details of chief investigator and the number of users are included in this appendix.

Table B.1: Projects using NPSF compute time

Institution	Project	Research Field	Chief Investigator	No. of users
ABV-Indian Institute of Information Technology and Management, Gwalior.	High energy density Supercapacitors and Effective Gas/Chemical/Bio-Sensors using 2D/1D Materials.	Material Sciences	Dr. Anurag Srivastava	4
Ahmednagar College, Ahmednagar.	To study the propertiees of layered structures and effects of doping there in using density functional theory	Atomic & Molecular Sciences	Dr. Pradip B. Shelke	1
Assam University , Silchar.	Quasiparticle band gap, vibrational and transport properties of some one and two dimensional nanosystems.	Chemical Sciences	Dr. Utpal Sarkar	1
Bharat Petroleum Corporate Research and Development Centre, Noida.	Development of the computational model to simulate the dynamics of the gas liquid flow in a scaled-down model of cross -flow reactor used in Hydro processing Applications.	Computational Fluid Dynamics	Dr. Biswanath Saha	2
Center for Modeling and Simulation (CMS), SP Pune University, Pune.	The prime objective of my project is to study the effect of defects on thermal transport and electronic transport of advanced materials using a novel atomistic approach.	Material Sciences	Dr. Ankita Katre	1
	First-principles investigation of semiconductor nanostructures.	Material Sciences	Prof. Anjali Kshirsagar	2
	Electronic Structure of novel materials.	Material Sciences	Dr. Bhalchandra S. Pujari	1

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Table B.1 – *Continued from previous page*

Institution	Project	Research Field	Chief Investigator	No. of users
Central University of Himachal Pradesh , Shahpur, Himachal Pradesh	To study the Vander Waals (vdw) heterostructures of borophene with 2D layered materials for exploring next generation electronic devices	Material Sciences	Dr. Jagdish Kumar	2
Central University of Rajasthan, Kishangarh,Rajasthan.	Ab initio Molecular Dynamics simulation of Ionic Liquid doped Polymer Electrolyte Membranes and Platinum Electrode Interface	Material Sciences	Dr. Anurag Prakash Sunda	1
Central University of South Bihar, Patna.	Molecular Dynamics study of thermo-stability of Archael protein.	*Uncategorized	Dr. Krishna Kumar Ojha	1
Centre for Gentic Manipulation of Crop Plants , University of Delhi South Campus,New Delhi.	Carrying out genome sequencing and phylogenomics analysis of Brassica species.	Bio Sciences	Prof. Akshay Kumar Pradhan	2
College of Engineering (COEP), Pune.	Blockchain Scaling and Measuring the Variation in Latency as the Network Scalability Changes.	Computational Sciences	Prof. Jibi Abraham	4
CSIR-National Chemical Laboratory (CSIR-NCL), Pune.	Elucidating the reaction mechanism of inorganic reactions (Computational Inorganic Chemistry)	Chemical Sciences	Dr. Kumar Vanka	2
	Investigations of thermoelectric performance of mixed metal organo halides: CH3NH3AB3 (A=Pb, Bi, Sb, B=I, CI, Br and mixture thereof)	Chemical Sciences	Dr. K C Bhamu	1

Continued on next page

Table B.1 – *Continued from previous page*

Institution	Project	Research Field	Chief Investigator	No. of users
Dibrugarh University, Dibrugarh, Assam.	Aerosol Radiative forcing over India(ARFI) and Atmospheric Trace gases, Chemistry, Transport and Modeling(AT-CTM).	Climate and Environment Sciences	Dr. Binita Pathak	3
Dr.Vijay Kumar Foundation, Gurgaon.	Research work on nano-materials.	Material Sciences	Dr.Vijay Kumar	8
Guru Gobind Singh Indraprastha University, New Delhi.	Study of thermoelectric properties of bulk nanostructured materials using Monte Carlo Simulations.	*Uncategorized	Dr. Sonnathi Neeleshwar	3
H.P.T Arts and R.Y.K. Science College, Nasik.	Computational Study on Graphene based NanoSheets for sensor applications.	Material Sciences	Dr. M.D. Deshpande	2
	Electronic Properties of TM doped ZnO Sheet: Density Functional Study.	Material Sciences	Dr. M.D. Deshpande	3
	Theoretical study of Structural, Electronic and Magnetic Properties of Nanomaterials.	Material Sciences	Dr. M. D. Deshpande	2
	Theoretical investigation of structural, electronic, magnetic and optical properties of undoped and doped iron oxide nanostructures.	*Uncategorized	Dr. Dattatraya Laxman Lalsare	1
Harish-Chandra Research Institute(hri), Allahabad.	Magnetic switching using 3d-organometallic molecule.	Materials Science	Prof. Prasenjit Sen	2
Himachal Pradesh University , Shimla.	In-plane heterostructure of Transition metal dichalcogenides.	Material Sciences	Prof. Raman Sharma	2

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Table B.1 – *Continued from previous page*

Institution	Project	Research Field	Chief Investigator	No. of users
	To study the effect of surface volume ratio and quantum confinement on the properties of Silicon nano wires.	Material Sciences	Prof. Raman Sharma	2
	To explore the properties of noble metal nanostructures in different phases computationally using DFT.	Material Sciences	Dr P.K. Ahluwalia	2
Indian Association for the Cultivation of Science(IACS), Kolkata.	Computational Investigations for the Linear and Nonlinear Optical Properties of Metal and Covalent Organic Frameworks: Applications for Detection of Molecules	*Uncategorized	Dr. Ayan Datta	1
Indian Institute of Astrophysics, Bangalore.	Numerical simulations of hydromagnetic turbulence from galaxies to the Sun	Astronomy and Astrophysics	Dr. Sharanya Sur	2
Indian Institute of Science Education and Research (IISER), Kolkata.	Dimeric stability of the NS1 protein of Zika virus.	Bio Sciences	Dr. Neelanjana Sengupta	2
Indian Institute of Science Education and Research (IISER), Pune.	Study of CdS and CdTeS quantum dots decorated on TiO2 nanowires.	Material Sciences	Dr. Prasenjit Ghosh	6
	Selective hydrogenation of acetylene on PdGa intermaetallic compounds(As per New TAS From: Selective hydrogenation of acetylene to ethylene on PdGa surfaces and clusters supported on MgO).	Material Sciences	Dr. Prasenjit Ghosh	6

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Table B.1 – *Continued from previous page*

Institution	Project	Research Field	Chief Investigator	No. of users
	Materails Modelling at Different Length and Time Scales.	Material Sciences	Dr. Mukul Kabir	4
	Point-Defects in Two-Dimensional Materials.	Material Sciences	Dr. Mukul Kabir	3
Indian Institute of Technology (IIT), Bhubaneswar.	Spin and quantum transport in covalently connected nanotubes.	*Uncategorized	Prof. Saroj Kumar Nayak	2
Indian Institute of Technology (IIT), Hyderabad.	First principles investigation of magnetic materials and superconductors	Material Sciences	Prof. Venkata Krishnan Kanchana	2
	First principles investigation of topological materials	Material Sciences	Prof. Venkata Krishnan Kanchana	2
	First principles investigation of thermoelectric materials	Material Sciences	Prof. Venkata Krishnan Kanchana	2
	Investigating seismic source physics inclusion into Engineering analysis of Built-Environment.	Geological Sciences	Dr. Surendra Nadh Somala	5
	Structure & dynamics of E.coli outer membrane proteins.	Bioinformatics	Dr. Thenmalarchelvi Rathinavelan	3
	Structure and dynamics of RMA duplexes comprising trinucleotide repeat expansion.	Bioinformatics	Dr. Thenmalarchelvi Rathinavelan	3
Indian Institute of Technology (IIT), Jodhpur.	Chemical Dynamics Simulations of Complex Organic Reactions: Mechanistic Insights and Microsolvation Effects.	Chemical Sciences	Dr. Manikandan Paranjothy	2

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Table B.1 – *Continued from previous page*

Institution	**Project**	**Research Field**	**Chief Investigator**	**No. of users**
Indian Institute of Technology (IIT), Kanpur.	Flow past a circular cylinder at high Reynolds numbers ∼O(10square 5) will be investigated.	Computational Fluid Dynamics	Dr. Sanjay Mittal	3
Indian Institute of Technology (IIT), Kharagpur.	Understanding of computational modeling of atomistic systems.	Computational Sciences	Dr. Puneet Kumar Patra	1
	Exploratory investigation on life of weld components in PFBRs	Atomic & Molecular Sciences	Prof. Baidurya Bhattacharya	2
Institute of Bioresources and Sustainable Development (IBSD), Imphal, Manipur.	Small dsRNA target prediction on human transcriptome using bioinformatics approaches.	Bio Sciences	Dr. K. Jeyaram	2
Institute of Nano Science and Technology (INST), Mohali.	Atomic scale design of novel nanomaterials for clean energy and devices.	Material Sciences	Dr. Abir De Sarkar	6
	Ab initio molecular dynamics (AIMD) Simulations.	Material Sciences	Dr. Md. Ehesan Ali	9
	Electronics and Thermal Properties of chalcogenide	Material Sciences	Dr. Chandan Bera	2
Interdisciplinary School of Scientific Computing, SP Pune University, Pune.	Piezoelectric materials are an integral part of ultrasound transducers, actuators, sensors, resonators etc. Such materials are mostly used in their doped forms to be used as anions or cations in various applications	Material Sciences	Dr. Vaishali Shah	3

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Table B.1 – *Continued from previous page*

Institution	Project	Research Field	Chief Investigator	No. of users
	Ab intio studies of doped GaNbO4 and TiO2 materials.	Material Sciences	Dr. Vaishali Shah	1
Jamia Millia Islamia University, New Delhi.	Collective Properties of Granular Media	*Uncategorized	Dr. Syed Rashid Ahmad	2
Kurukshetra University, Kurukshetra.	Simulations of rare earth free magnetic materials and hybrid organic-inorganic halide perovskites for photovoltaic applications.	Computational Sciences	Dr. Manish Kumar Kashyap	3
National Institute of Technology (NIT), Silchar.	Spectral element methods for elliptic and parabolic interface problems.	Computational Sciences	Dr. Pankaj Biswas	2
Osmania University, Hyderabad	Modeling & Simulations of Materials.	Material Sciences	Dr. Moumita Saharay	2
Panjab University , Chandigarh.	Superconducting parameters of the conventional superconductors are calculated theoretically using FP-LAPW method as implemented in ELK code.	Material Sciences	Prof. Ranjan Kumar	2
	Exploring half-Heusler Compounds for thermoelectric Applications.	Material Sciences	Prof. Ranjan Kumar	2
	Ab-initio study of 2 Dimensional Thermoelectric Materials.	Material Sciences	Prof. Ranjan Kumar	2
Pondicherry University, Pondicherry.	Study of correlation effects in heavy molecules and solids and its implications to parameters of fundamental symmetry violation	Atomic & Molecular Sciences	Dr. K. V. P. Latha	3

Continued on next page

Table B.1 – *Continued from previous page*

Institution	Project	Research Field	Chief Investigator	No. of users
	Monte Carlo Simulation of Lattice Polymers	*Uncategorized	Dr. S V M Satyanarayana	2
Sardar Vallabhbhai National Institute of Technology (SVNIT), Surat.	Novel perovskite-based solar cells: Investigation of potential properties using ab-initio approaches	Material Sciences	Dr. Yogesh Sonvane	5
SASTRA University, Thanjavur, Tamilnadu.	Hydrogen Storage on Alkali Metal Functionalized Porous Descrete Organic and Polymer Hosts for Onboard Utilization	Material Sciences	Dr. Venkataramanan N S	2
	Inclusion Complexes of Cisplatin and its Analogues	Chemical Sciences	Dr. A. Suvitha	1
St. Xaviers College, Ahmedabad.	Quantum transport in elemental doped boron nitride monolayer	Material Sciences	Dr. Sanjeev Kumar Gupta	1
UGC-DAE Consortium for Scientific Research, Indore	First Principles Modeling of Dzyaloshinskii-Moriya Interactions in Magnetic Multilayers	Material Sciences	Dr. Rajamani Raghunathan	1
UM-DAE Centre for Excellence in Basic Sciences, Mumbai.	A well -defined structure of a protein has so far been considered to perform its functions.	Chemical Sciences	Dr. Sunita Patel	1
University of Hyderabad, Hyderabad.	Carbondionide capture and storage: Exchange with methane in clathrates.	Chemical Sciences	Dr. Manju Sharma	1
University of Madras, Chennai.	Studies on hybrid organic-inorganic Halide Perovskite using first-principles density functional theory	Computational Sciences	Dr. R. Radhakrishnan	1
University of Mysore, Mysuru.	Studies of proteins using Molecular Dynamics Simulations.	Atomic & Molecular Sciences	Dr.S. Krishnaveni	2

Continued on next page

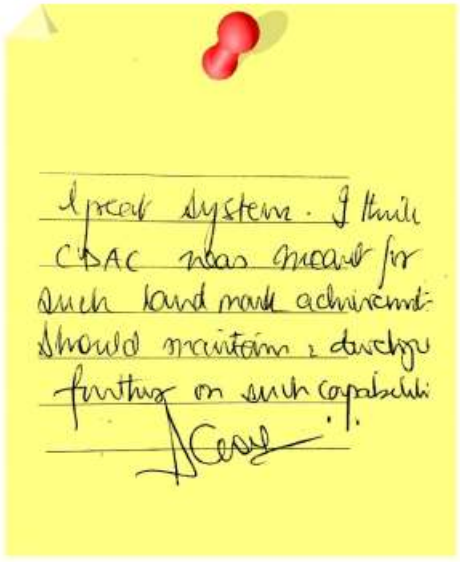
Table B.1 – *Continued from previous page*

Institution	**Project**	**Research Field**	**Chief Investigator**	**No. of users**
Visvesvaraya National Institute of Technology (VNIT), Nagpur.	First priniciple study of some topological materials	Material Sciences	Dr. Poorva Singh	2
Whistling Woods International Institute (WWII), Mumbai.	Rendering some of the shots for 15 Minute Short Film on PARAMYuva-II GPUs	Computational Sciences	Ms. Anuradha Bhatia	2

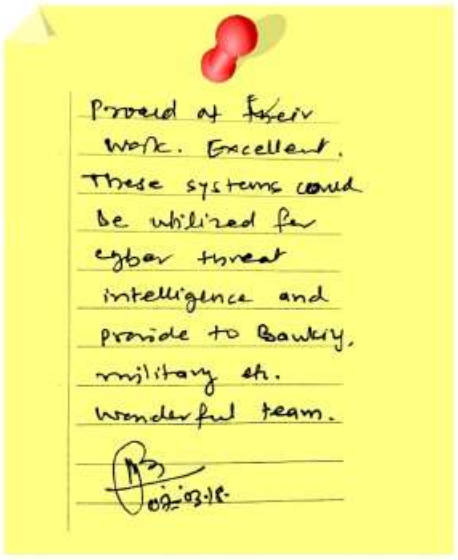
*Uncategorized : Projects for which no information on research field was provided by their respective Chief Investigators

Appendix C

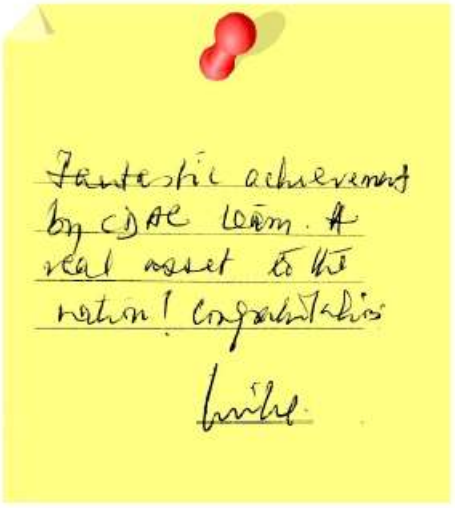
Visitors Quotes



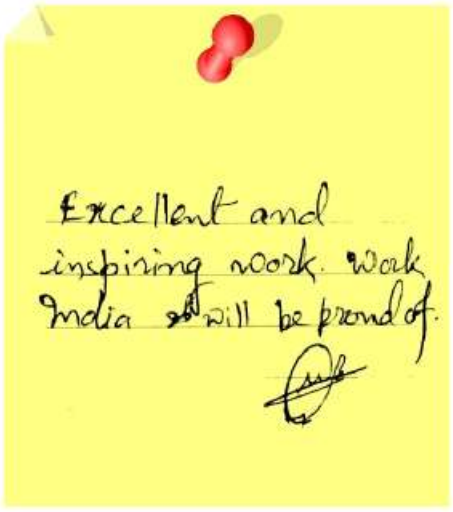
Mr. S. Goel , J.S, Meity



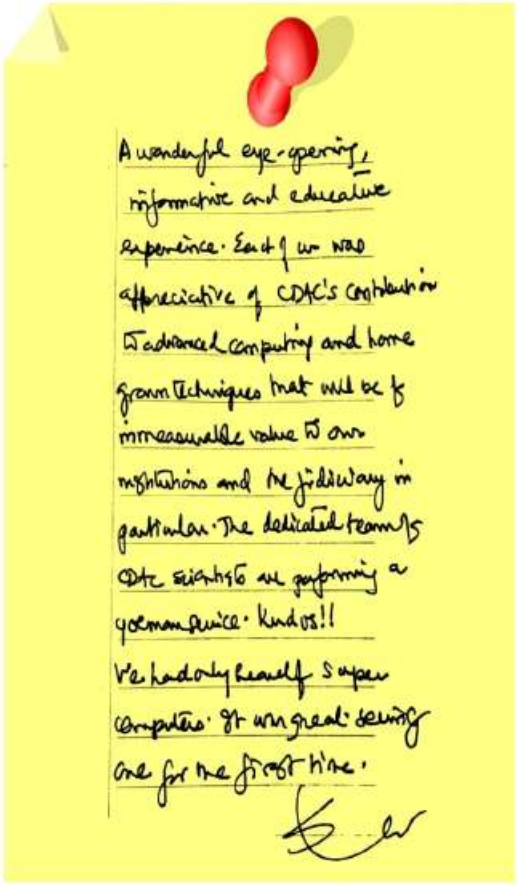
Mr. Makarand. B. Kedare, DGM(IT Innovations), SBI



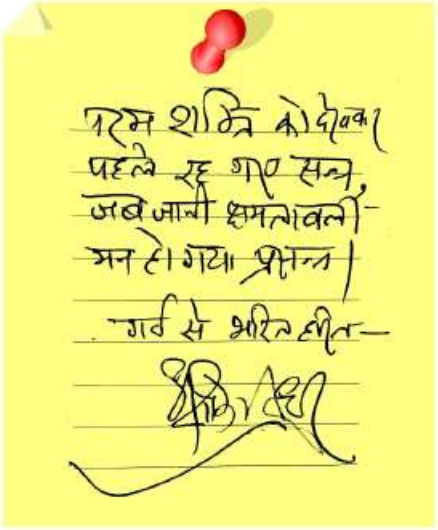
Ms Anuradha Mitra,
Member(Finance), Meity



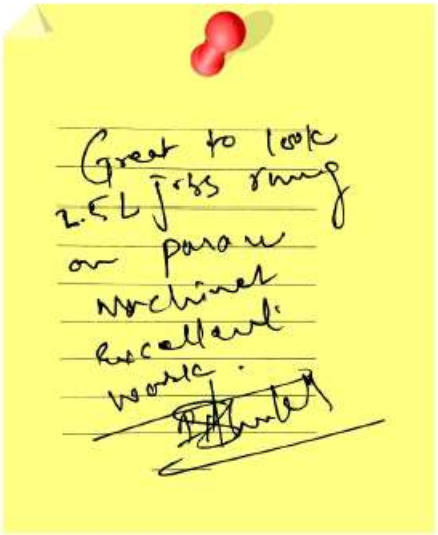
Wg cdr M.M Ingale



Judges of the High courts of Mumbai, Madhya Pradesh, Punjab, Haryana and Delhi

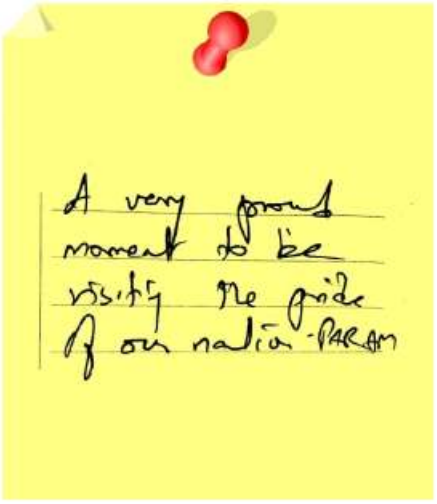


Mr. Ashok Chakradhar, Hindi Poet & former HOD of Hindi at Jamia Milia Islamia University, New Delhi

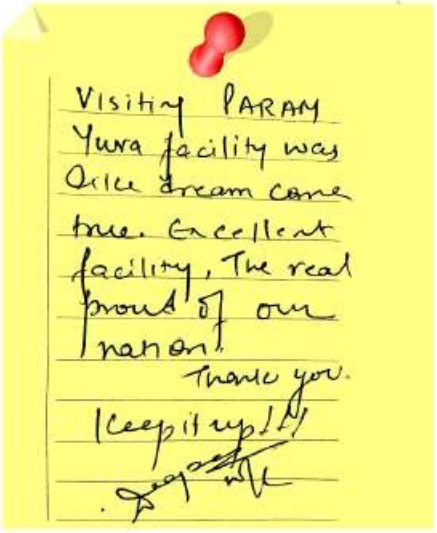


Mr. Israr Sheikh, Mr. Narsimha Ranganathan

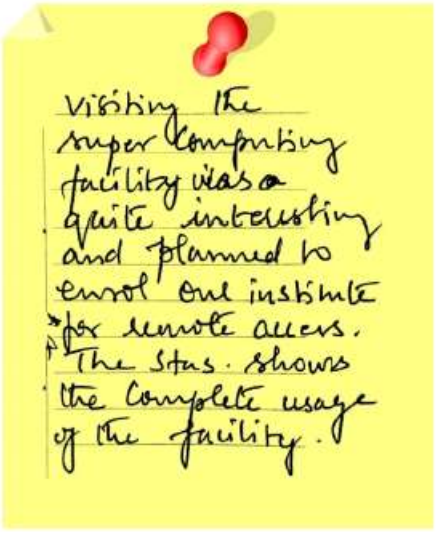
Prof. Vladimir Voevodin, Moscow State University



Prof. Ramesh Loganathan, IIIT, Hyderabad



Mr. Deepak Prasad, SSE (SIM) SDI, AF



Prof. R. Jagadeesh Kannan, VIT University, Chennai

Seeing India's most efficient HPC was a special treat for a former Fortran programmer now working in energy efficiency! Keep up your amazing work!

Mr. R. Laemel, Senior Associate, Rocky Mountain Institute, Basalt, USA.

We are proud to have our association with C-DAC. I am happy to be here today & see the supercomputer developed by the country kept in this premises. My best wishes for taking this mission forward.

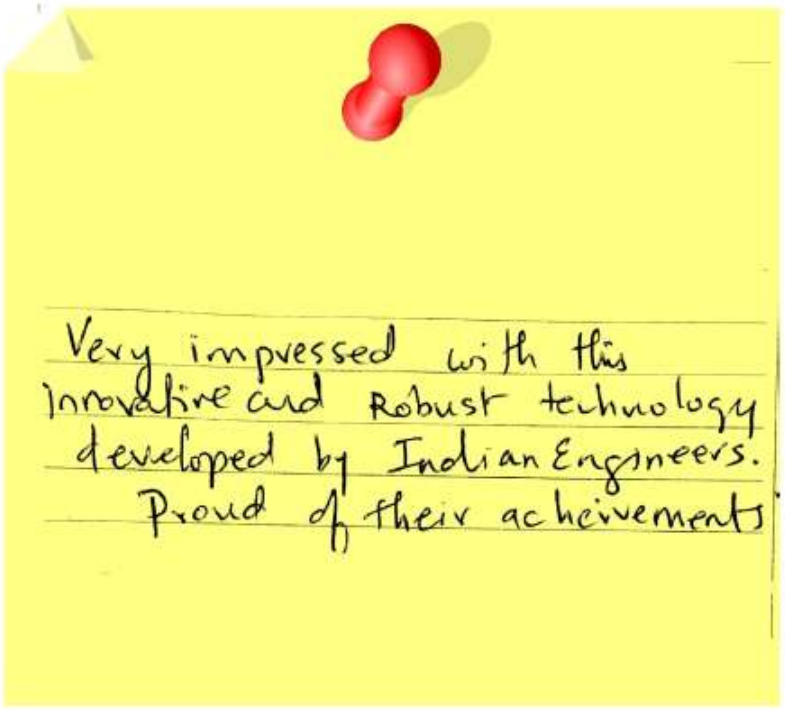
Mr. Sunil Barthwal, IAS, CPFC, EPFO & Additional Secretary to Govt. Of India

It's a technological marvel. It will help nation move up the technology ladder.

Dr. P. K. Khosla, ED, CDAC Mohali

Excellent facility Created. Must be made available to all NKN Institutions for R&D Activities. Infact Some of Supercomputer should be made available to foreign institutions for R&D.

Mr. Vinay Thakur, Director, NEGD , MeitY



Prof. Venkatesh Raghavan, Osaka State University.

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Appendix D

Picture Gallery

Visit to NPSF by Ms. Anuradha Mitra, AS & FA, Meity, New Delhi.

Visit to NPSF by Joint Committee of Hon'ble Judges of High Court.

Visit to NPSF by Parliamentary Committee on IT.

Visit to NPSF by Uzbekistan Delegate.

Visit to NPSF by Joint Committee of Hon'ble Judges of High Court.

NPSF members during National Science Day event, C-DAC, Pune.

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Nisha Agrawal

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Saurabh Muley
Shivam Nirhali

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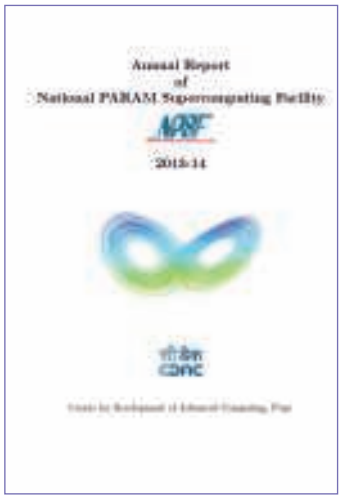

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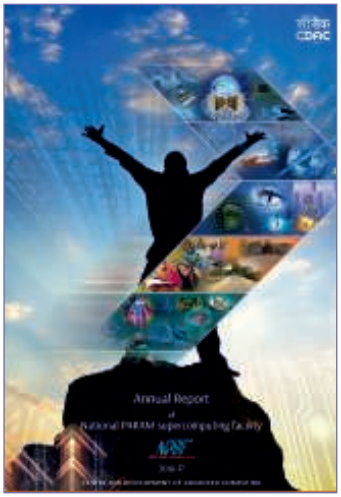

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