National PARAM Supercomputing Facility

Version 2.0

ANNUAL REPORT 2019

CENTRE FOR DEVELOPMENT OF ADVANCED COMPUTING

Cover Note

Dear Reader,

Taking forward tradition, NPSF is proud to presents Annual Report for the year 2019. The information in the report is providing 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 specially the scientific outcome of utilization, we have participation from NPSF's user community wherein information regarding PhDs, Publications and Work Reports are included verbatim.

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

Happy Computing!

Regards
NPSF

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आवरण पत्र

प्रिय पाठक गण,

अपनी परंपरा को आगे बढ़ाते हुए, एनपीएसएफ वर्ष 2019 की वार्षिक रिपोर्ट प्रस्तुत करते हुए गौरवान्वित महसूस कर रहा है। हमारे प्रदर्शन के साथ ही, भारत में सामान्य रूप से एचपीसी गतिविधियों को समझने और विश्लेषण करने के अभिप्राय के साथ, एनपीएसएफ की एचपीसी सेवाओं का उपयोग करते हुए, किए गए कार्यों की गुणात्मक और परिमाणात्मक दोनों पहलुओं को इस रिपोर्ट के माध्यम से प्रस्तुत किया गया है। परिमाणात्मक भाग के रूप में, वर्ष के दौरान की गई प्रणाली उपयोगिता कार्यों को शामिल किया गया है, और इसके माध्यम से भिन्न-भिन्न उपयोगिता पहलुओं के समावेशी दृष्टिकोणों को प्रस्तुत किया गया है। गुणात्मक भाग की बात करें, तो विशेष रूप से उपयोगिता के वैज्ञानिक परिणामों को शामिल किया गया है, जहां हमने एनपीएसएफ उपयोगकर्ता समुदाय की ओर से प्रतिभागिता की है। साथ ही इसमें हमारे द्वारा पीएचडी, प्रकाशन और कार्य रिपोर्टों के संबंध में शब्दशः जानकारी को शामिल किया गया है।

इस रिपोर्ट तथा एनपीएसएफ पर आपकी अमूल्य प्रतिक्रया, सुझावों आदि से हमें अति प्रसन्नता होगी। आप, अपने सुझाव आदि हमें npsfhelp@cdac.in पर ईमेल कर सकते हैं।

शुभ कंप्यूटिंग, सशक्त कंप्यूटिंग!

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 1st 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 93%. For all the successive years 2013 onwards, each year NPSF saw the ever increasing demand for the HPC resources with a record execution of >444 thousand HPC jobs under 330 Projects submitted by 1100+ users from across 120+ 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 Brahma, 850 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 is 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

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

Message from Executive Director

Since its inception in year 1998, National PARAM Supercomputing Facility (NPSF) has contributed significantly in solving complex computational problems of importance to nation from scientific and academic community. During its 22 years of operations of serving the nation, NPSF has evolved from 100GFLOPS PARAM 10000 Supercomputer to 524TFLOPS PARAM Yuva II Supercomputer.

I congratulate all members of NPSF team for their continuous and tireless contribution in providing support to 1193 users from 121 R&D and academic institutions that have used PARAM Yuva II for their scientific, research and development work. The success of the facility is clearly indicated by its consistent usage of above 95% along with its contribution in 64 publications and 15 PhD theses.

The year 2019 has been a great year for C-DAC in which the knowledge and expertise of more than two decades in high performance computing has helped C-DAC strengthen the Nations computational resources even further.

With the knowledge and expertise gained over decades of experience, NPSF has a critical role to play in forthcoming challenges in High Performance Computing, Artificial Intelligence and Exascale Computing. I extend my best wishes and whole hearted support to NPSF and its user community for all their future endeavors and achievements.

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

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

Message from Head of Department

The NPSF annual report has always represented a milestone and a connection between what has been achieved in the previous year. We are pleased to present this look back at our activities over the past 12 months, which were marked by successes despite of a major breakdown in our storage subsystem.

During the past year, the NPSF user community has crossed 1180+ and the total number of jobs executed has risen to 4,00,000+ with above 95% of CPU utilization.

Between 08-Apr-2019 to 22-Jul-2019, the facility was not operational due to storage sub-system failure, inconveniencing our users. The storage is now replaced, and the six-year-old facility has got a new lease of life, and is now fully functional and available to users again.

I hope you find this Annual Report useful and insightful and share my excitement about the potential for HPC to tackle some of the greatest challenges facing our nation and the world.

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

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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 was 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, which was 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

Two 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	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.

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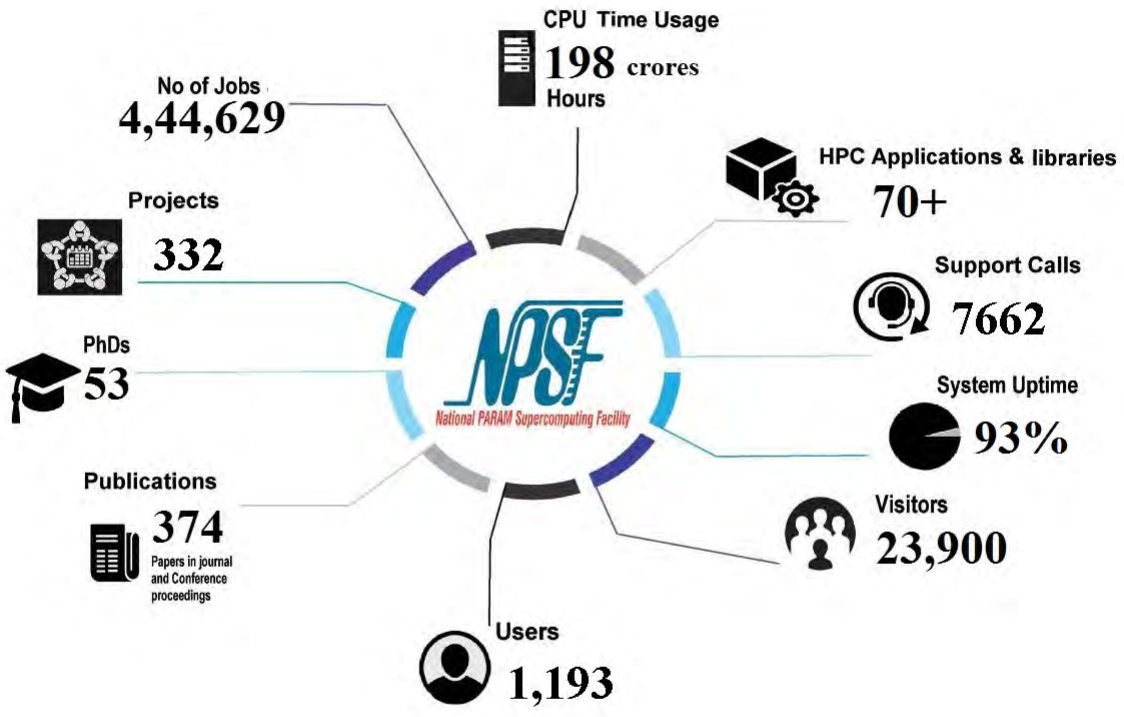
NPSF in Last Seven Years

Below are some of the NPSF statistics of last seven years i.e Year 2013-19.

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



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2.1 NPSF in 7 years

C-DACs National PARAM Supercomputing Facility (NPSF) was established in March 1998 with the mandate to offer state-of-the-art High Performance Computing systems to various institutions and industries that need such a facility to process their diverse applications and resources, also to help them with the know-how and usage of such systems and proliferate HPC awareness in the country.

Major Events

- As part of Provisioning of hybrid technologies in National PARAM Supercomputing Facility and C-DACs Terascale Supercomputing Facility - A step towards Next Generation HPC project, PARAM Yuva II system was launched in February, 2013. The system performs at a peak of 524 TFLOPS, about 10 times faster than its predecessor i.e. PARAM Yuva. PARAM Yuva II relies on Intel Xeon Phi for its computing power, thus making it energy efficient than its predecessor thus boosting the Flops per Watt index.
- The increase in peak compute power from 54 TeraFLOPS to more than half a PetaFLOPS is achieved without any increase in the electrical power and cooling required for the facility.
- Also, with this launch, C-DAC became the first R&D institution in India to cross the 500 TF milestone.
- Meticulous planning and co-ordination, consistent efforts and use of expertise gained over years helped in commissioning the in record time of 21 days and the system was then offered as resource to the HPC community.
- Benchmarking exercise for Top500 ranking was done for PARAM Yuva II system and achieved sustained performance of 386.7 TeraFLOPS and was ranked 69th in the June 2013 Top500 list.
- Energy consumed by supercomputers is measured at various Levels - L1, L2, and L3 - for purpose of reporting as part of Green500 list. As the level increases, accuracy and rigor of measurement exercise also increases. It is noteworthy that NPSF team has carried out Level 3 benchmark and C-DAC became the second organization worldwide to have carried out the Level 3 measurement of Power versus Performance for the Green500 List. C-DAC achieved a significant milestone with PARAM Yuva II being ranked 1^{st} in India, 9^{th} in the Asia Pacific Region and 44^{th} in the world among the most power efficient computer systems with performance of 1,760.20 Mega Flops (MFs) per Watt as per the Green500 list released in November 2013
- In order to strengthen the security and accessibility of the PARAM Yuva II system, the system software architecture was re-architected and entire system was reinstalled with near diskless, read-only setup.
- The security has been enhanced at various levels like data security, cluster level security, system level security, login access control and perimeter level security
- Revamping of cluster partitions was done in order to ensure optimal resource utilization and cater to the specific need of resources by group of users
- As an effort to apprise Chief Investigators (CI) of projects in NPSF, and also to serve as usage charges levied (not commercial), NPSF has started raising invoices for monthly CPU time utilization

- Space Application Centre, ISRO has used NPSF PARAM Yuva II system extensively for their daily operational jobs run for consecutive 3 years with 99.4% of the days successful job runs. The jobs have been managed to run in the maintenance period as well. NPSF team received acknowledgement from ISRO for availability and maintenance of the resources and support provided.
- 2018 was a proud year for us, as the system uptime was maintained to 99.95% which is the highest of all the years of NPSF. The efforts made by team to keep facility up and running all the time had shown the results.

System Management and monitoring

To test various policies and configurations before deploying on the actual PARAM Yuva II system, a similar setup has been created so that any evaluation of installation, configuration change or policy implementation can be tested before being placed into production

Remote management was enabled for all the nodes in-order to manage them remotely even when OS is not booted or node crashed, also to perform power ON/OFF/Recycle remotely

The PARAM Yuva II ecosystem is being monitored closely with the help of monitoring tools. Alerts are also in place to catch the attention on priority NPSF Web Portal: Feature rich and user friendly

NPSF web portal has been in place. It also serves as collaborative environment for NPSF user community.

On the development front, development/customization and installation of required tools for efficient use of the system and ease of monitoring and management of the facility has been done. This majorly included power aware scheduling, customized monitoring tools, customized resource manager and scheduler, performance data collection framework and many other tools and services. Automation of the many day to day tasks is also done.

System utilization and Usage Policies

- Since the facility is shared by more than 1100 users across India, adequate mechanisms are put in place to ensure maximum throughput and optimal resource usage of the systems. The policies are made based on the systems capabilities, targeted use and user demand for the resource. The policies are periodically monitored and changed if necessary.
- Dedicated Slot Booking Facility: Online Dedicated Slot Booking Facility was in place to address the need for the dedicated resources by users. The dedicated slots have been provided to the users at regular intervals. Several users are greatly benefitted by the use of DSBF.
- For processing of large number of cores (512 to 1024) jobs with less wall time, a new execution queue BURSTq was introduced on 9th Sept., 2016. The jobs requiring more than 512 and less than 1024 cores for maximum 17:55:00 Hrs wall time jobs were made to route to this queue. Introduction of this queue helped a lot for processing of BIG jobs.
- The usage reports are generated on a monthly basis and help us to understand the usage patterns, which help us in fine tunning the usage policies.

User Support

Keeping in view the practice followed worldwide, a scheme, called the Technical Affiliation Scheme (TAS) is in place with an objective of encouraging the potential users of high performance com-

puting resources in a cost-effective way and also provides technically congenial environment to the researchers using NPSF. NPSF team has been supporting large pool of HPC users belonging to various application domains and profiles via e-mail, chat, telephonic support, sharing the user terminal and in person.

Workshops, Lectures and Talks

From last 3 years, NPSF team members are engaging themselves in delivering lectures, oversee and guide during lab practice sessions and, conducting end module exams, for PG Diploma on HPC System Administration (HPC-SA), under Advanced Computing Training School (ACTS), C-DAC. This is 6 monthly, twice in a year activity.

In the last 7 years, NPSF team members have organized 9 workshops and delivered more than 20 talks in different forums.

Breakdowns

PARAM Yuva II cluster is being managed without any AMC from last 3 years. NPSF team has been maintaining the cluster on best effort basis. There have been breakdowns in the facility due to failures in IT and non-IT infrastructure. In the recent past, NPSF PARAM Yuva II services were largely affected due to failures in the IT infrastructure, mainly due to storage failure. In addition to the failures in the IT- Infrastructure, there have been unplanned service breakdowns due to non-IT infrastructure failures as well, mainly due to power sub-system failure. The total downtime in the last 7 years is 7% out of which 50 % of the downtime has been added in this year which is the downtime accounted due to storage subsystem failure.

Acknowledgement

The activities of the National PARAM Supercomputing Facility were supported by the grant-in-aid financial support from MeitY, Ministry of Communications and Information Technology. We gratefully acknowledge the funding of these projects by MeitY,

Also, we express our sincere gratitude to the members of the PRSG committees who have guided and supported the activities of NPSF.

Our sincere thanks to our Director General, Executive Director and Head of the Department who have made sure that NPSF continue to offer services in spite of funding issues.

Finally, we acknowledge support received from ever growing NPSF user community to make this journey successful.

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2.2 7 years Statistics

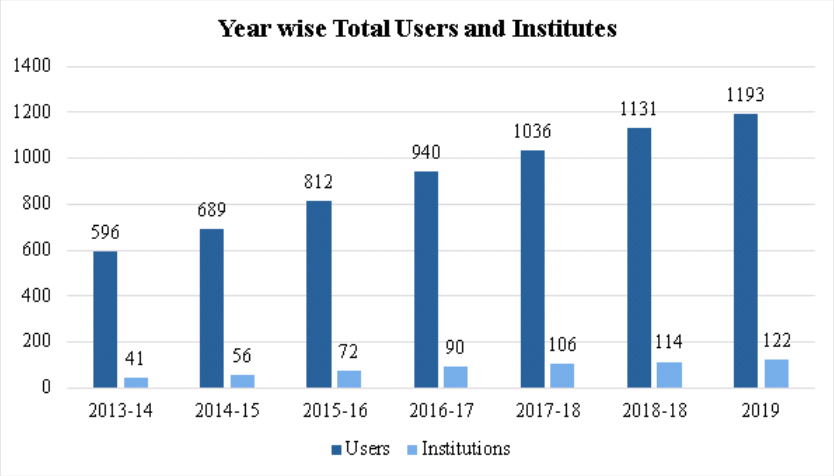


Table: Year wise total users and institutions

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
2019	1193	122

The above bar graph shows growth in the count of NPSF users and institutes affiliated to NPSF. It noteworthy that the number of users have doubled and number of institutions have tripled in the last 7 years.

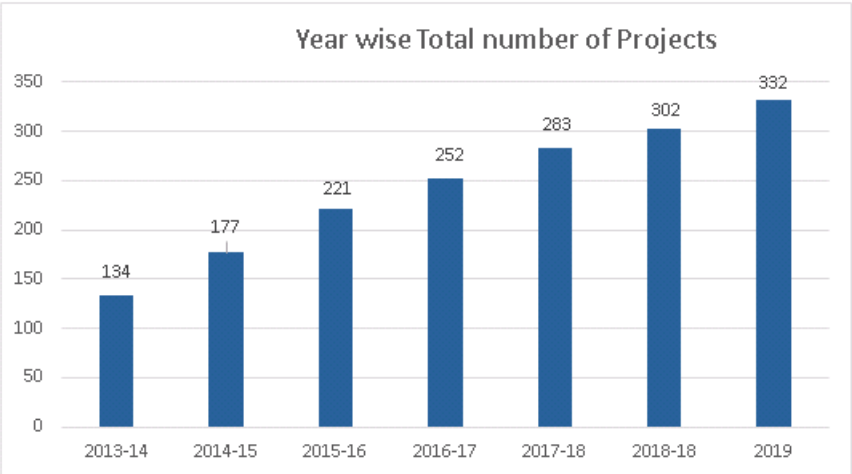


Table: Year wise total number of projects

Year	Number of Projects
2013-14	134
2014-15	177
2015-16	221
2016-17	252
2017-18	283
2018	302
2019	332

In the above bar graph, substantial growth in the number of projects registered with NPSF in the last 7 years.

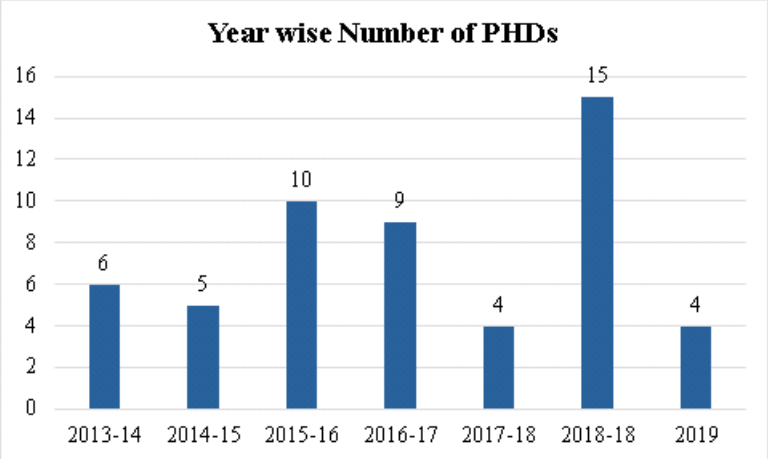


Table: Year wise number of PhDs

Year	Number of PhDs
2013-14	6
2014-15	5
2015-16	10
2016-17	9
2017-18	4
2018	15
2019	4

Above graph shows the count of PhDs completed using NPSF PARAM Yuva II system. In the last 7 years, total 53 PhDs have been completed using NPSF PARAM Yuva II system. This also includes 4 PhDs awarded last year.

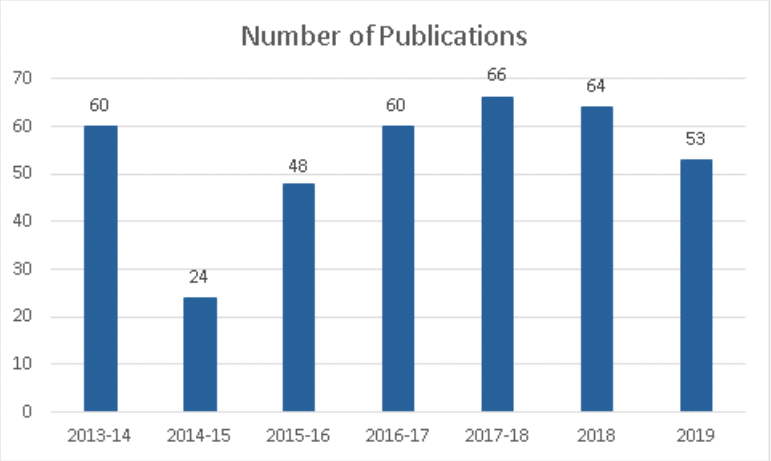


Table: Year wise number of publications

Year	Number of Publications
2013-14	60
2014-15	24
2015-16	48
2016-17	60
2017-18	66
2018	64
2019	53

NPSF users publish the publications in the journals where they duly acknowledge the NPSF PARAM Yuva II system. The total number of publications using the system is 374 and every year except 2014-15, nearly fifty or more publications are published in the reputed journals.

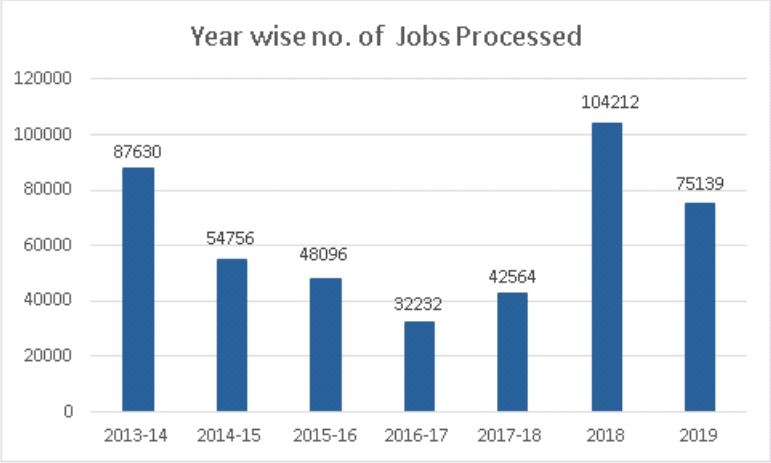


Table: Year wise number of jobs processed

Year	Number of jobs processed
2013-14	87630
2014-15	54756
2015-16	48096
2016-17	32232
2017-18	42564
2018	104212
2019	75139

Total number of jobs processed using NPSF PARAM Yuva II system is near to 4.5 Lac in the last 7 years. In spite of 105 days long maintenance, the count of the jobs processed has been above 80,000.

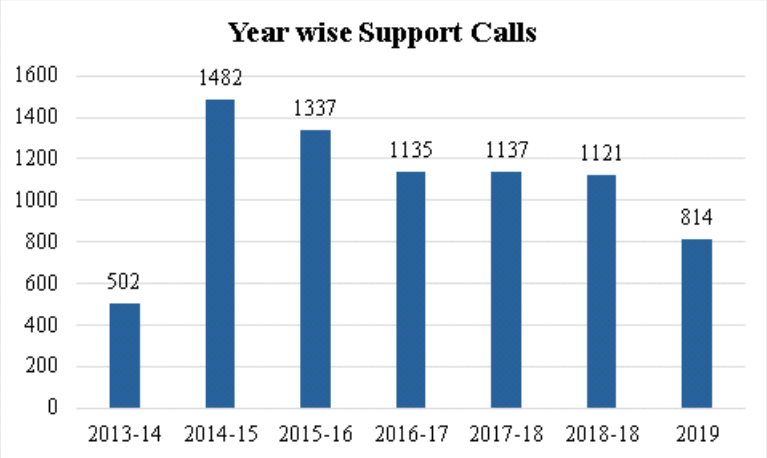


Table: Year wise number of support calls

Year	Number of support Calls
2013-14	502
2014-15	1482
2015-16	1337
2016-17	1135
2017-18	1137
2018	1121
2019	814

Above graph shows Year wise number of support calls raised by NPSF users over e-mail for the help they require while on-boarding / using the system. The calls are duly resolved and users are notified over e-mail about the resolution. Around 1500 support calls are raised over e-mail till 2019.

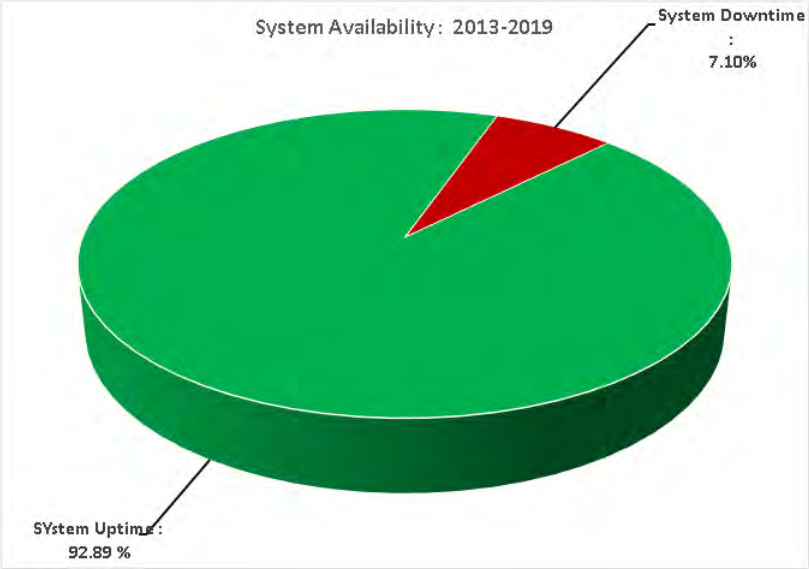
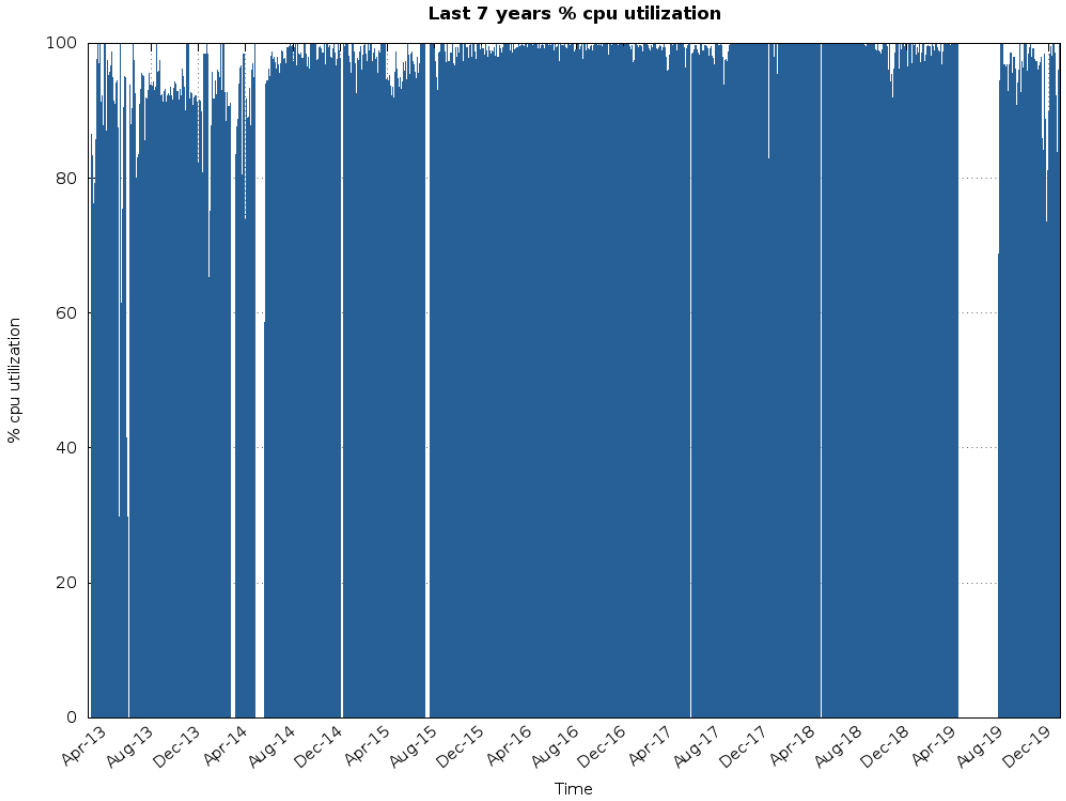


Table: System availability

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
2019	70.31	29.69

The pie chart is an indicator of system uptime (availability) which one of the most important aspects of HPC facility. NPSF PARAM Yuva II system has 92.89% of the uptime. Till last year, the total uptime was 96.65%, but the uptime has reduced to 92.89% due to 105 days long maintenance happened in 2019 that was caused by storage subsystem failure.



% cpu utilization is calculated as % of cpu cores used out of available cpu core. This utilization is recorded every minute in the database. The above GNU Plot shows utilization of 90% and above most of the time over the period of 7 years. This graph is also indicative of very high utilization of the system consistently. The gaps in the plot are indicative of maintenance period of the system and few times, non-availability of the stats.

3

Highlights

1. NPSF HPC services were interrupted due to failure in storage subsystem on 1^{st} Jan, 2020 .Emergency maintenance was carried out to correct the fault and lasted around 6 hours , after which services were restored and system was made online for job execution.

2. As part of C-DAC's tradition, NPSF team participated to showcase NPSF during National Science Day celebration at C-DAC, Pune, 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.

3. Apart from NPSF operations, team members are faculty of Advanced Computing Training School (ACTS), C-DAC for PG Diploma course titled HPC System Administration (HPCSA). 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.

4. As an effort to apprise Chief Investigators (CI) of projects in NPSF, and also to serve as usage charges levied (not commercial), NPSF has been raising invoices for monthly CPU time utilization. In 2019, total 1370 invoices have been raised against consumed CPU Time of 34169482 CPU Hours. The e-money equivalent of the consumed CPU Time is 110823840.50 debit units.

5. NPSF PARAM Yuva II services were largely affected due to failure of the storage system at NPSF. The system was not available for use for 105 days.

We have been handling the 3 tier HPC storage i.e. home area, scratch area and Tape based backup since it was commissioned in 2010. The appliance based storage has been maintained without AMC since last 5 years and the encountered issues have been fixed based on our experience gained. Due to non-availability of spares, we have kept 10% components as spares from the available storage by compromising on the capacity offered to the users.

On 8^{th} April, 2019, the issue of simultaneous and multiple hard disk failures in the home area storage subsystem occurred, that caused the filesystem to go unresponsive (I/O errors). The PARAM Yuva II system was taken in to emergency maintenance due to non-availability of the storage. All the possible efforts were made to recover the filesystem which unfortunately did not succeed. Even the paid call raised with OEM was also not useful. Re-commissioning exercise of the storage with the existing hardware was carried out where, while recommissioning, multiple hardware components started failing and the re-commissioning could not happen.

Finally, the 200 TB storage was arranged and was configured to serve as the home area of the PARAM Yuva II users. The system configuration was restored from backup and data of the users was restored on demand on a chargeable basis. The scratch filesystem was decommissioned. The system with configured storage was released on 22nd July, 2019 for use.

6 Ms. Nisha Agrawal delivered invited talks and assisted in hands on session in Five day Faculty Development Program (FDP) on High Performance Computing (HPC) at Walchand College of Engineering, Sangli, held on July 15-19, 2019.

7 NPSF system suffered from unforeseen power outage issue due to heavy rains on 5th August, 2019. The system was restored after restoration of power (after 30 hours).

8 Mr. Puneet Bakshi, Mr. Pankaj Dorlikar and Ms. Nisha Agrawal have delivered lectures on HPC storage technologies and HPC system monitoring to National Investigation Agency (NIA) officers as part of their 15 days system administration training at C-DAC Pune during September 2019.

9 Ms. Nisha Agrawal mentored Institute of Plasma Research (IPR) team at GPU Application Hackathon 2019 (GAH-2019), 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 14th 18th of September, 2019.

10 NPSF team organized one day internal workshop on Seeking inputs towards the planning of Next Generation HPC system at C-DAC during October 2019.

11 NPSF services were affected due failure of the InfiniBand FDR Switch on 18th September, 2019 and 30th December, 2019. The system was restored back to service 19th September, 2019 and 31st December, 2019 respectively.

12 DGX1 demo systems commissioned at NPSF were used by participants for running their models on GPU accelerators during AI Hackathon organized by C-DAC Pune from 26th September, 2019 to 30th September, 2019.

13 NPSF team is working on offering the large capacity and high bandwidth storage to the NPSF user community on requirement basis. The storage systems are being setup at NPSF under C-DACs initiative of establishing Storage Incubation & Experience Center. The goal is to demonstrate the applications scalability and associated benefits, both in terms of advancements in respective field of research and societal impact.

4

Statistics

In Year 2019: Users added: 62; Institution added: 08; Jobs processed: 75,139

4.1 System

System availability

The pie chart is an indicator of system uptime (availability) which is one of the most important aspects of HPC facility. NPSF PARAM Yuva II services were largely affected due to failure of the storage system at NPSF. Apart from this, NPSF services were affected due failure of the InfiniBand FDR Switch. These failures have impacted on the overall availability of the system and services to the user community. It can be seen that the system availability has reduced to 70.31% from 99.95%, as compared to last year one.

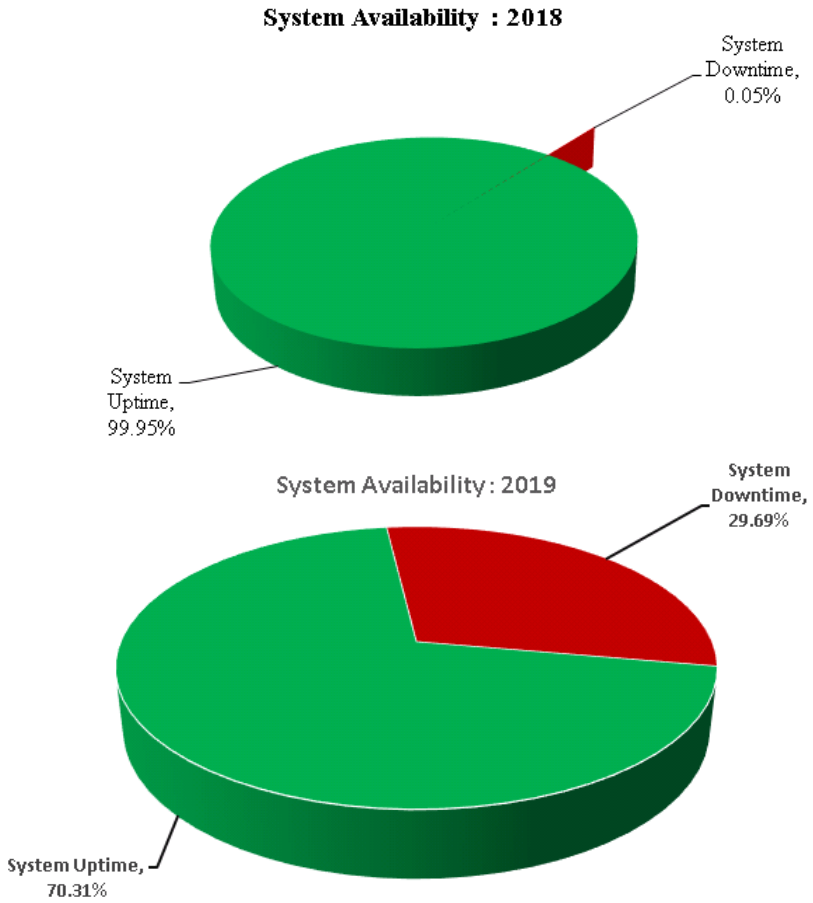
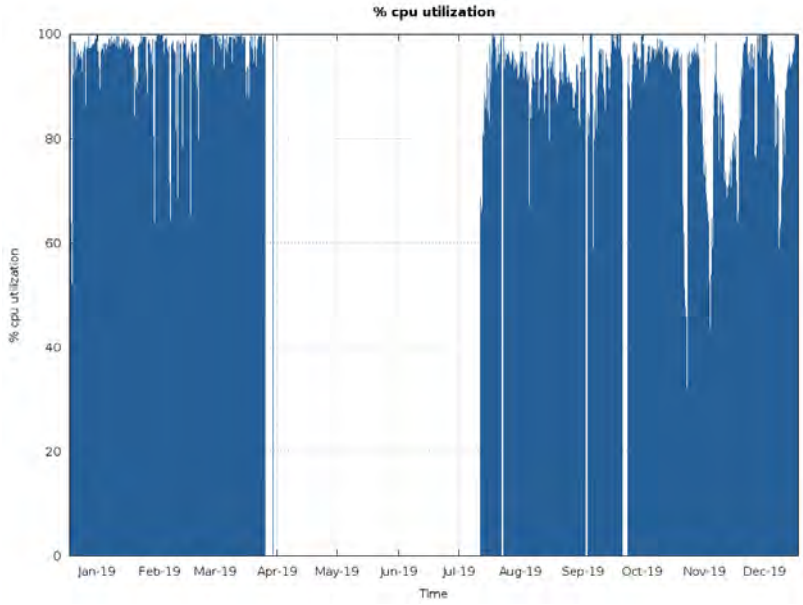


Table: System availability

Duration	Total Time	Downtime
1 Jan'18 - 31 Dec'18	365 Days (total : 8760 Hours)	0.21 Days (5 Hours, 13 Minutes)
1 Jan'19 - 31 Dec'19	365 Days (total : 8760 Hours)	108.35 Days (2600 Hours, 34 Munites)

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 indicated by the scheduler. This utilization is recorded every minute in the database. From the above GNU plot, It can be seen that the system utilization most of the times remained above 90% throughout the year. The gaps in the plot are indicative of non-availability of the system and few times, non-availability of the data. The gap seen between 8th april 8 to 22nd July, 2019 is the indicator of non-availability of the system due to failure of the storage system at NPSF



CPU time utilization w.r.t. job sizes

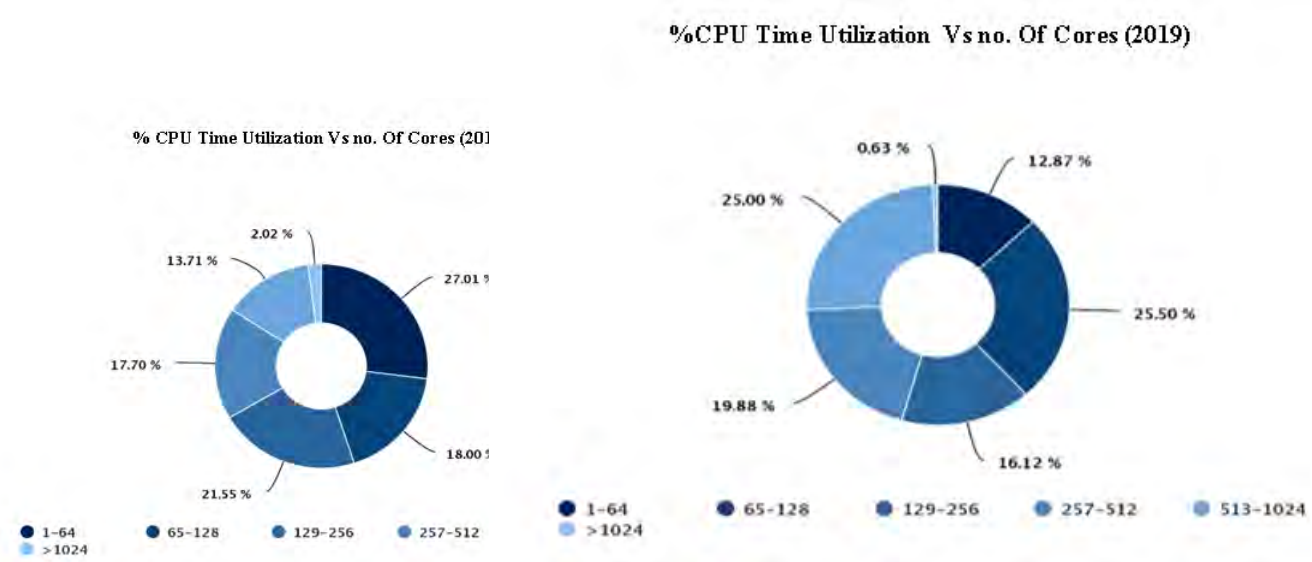


Table: CPU time utilization w.r.t. job sizes

	CPU time utilized (in seconds)	
Job Sizes	**2018**	**2019**
1-64	38430639920	17353205383
65-128	25613338018	34370568320
129-256	30660088882	21729859504
257-512	25185869864	26800724448
513-1024	19504730320	33704459698
>1024	2872174464	845818160

Above doughnut indicates % distribution of CPU Time among different job sizes (binned by number of cores). It can be seen that there is 13% increase in use of CPU Time by big jobs (jobs requiring more than 64 cores).This is also indication of increase in % of capability computing.

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

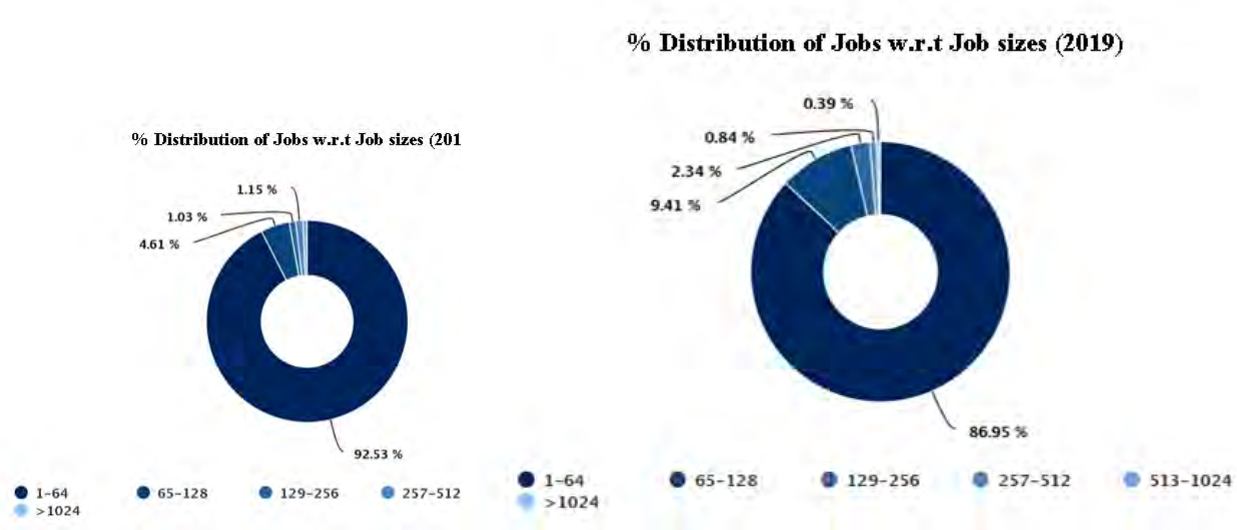


Table: Distribution of jobs w.r.t. job sizes (in seconds)

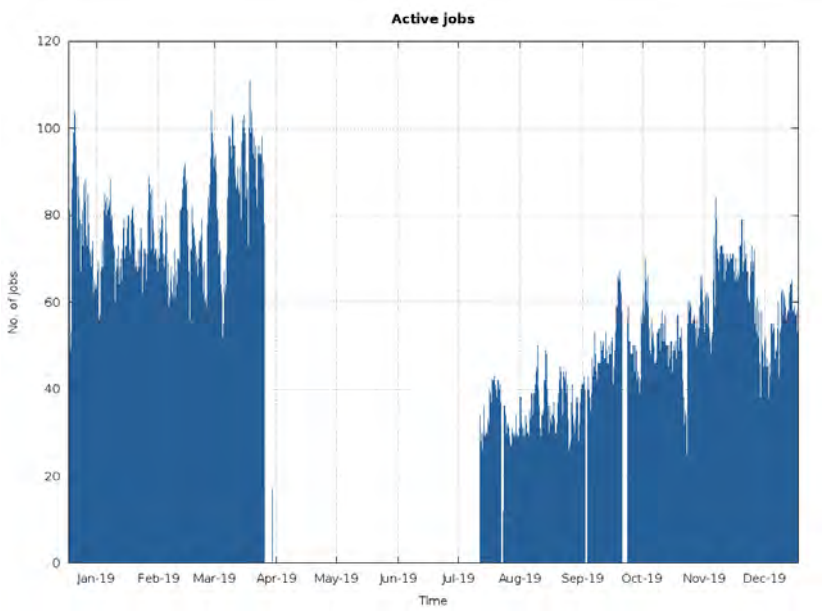
	Job Count	
Job Sizes	**2018**	**2019**
1-64	96430	70566
65-128	4807	7634
129-256	1077	1901
257-512	1197	680
513-1024	684	318
>1024	15	62

Above doughnut indicates % distribution of number of batch jobs binned by number of cores. The percentage of number of big jobs (jobs requiring more than 64 cores) has increased from 7% to 12% from last year.

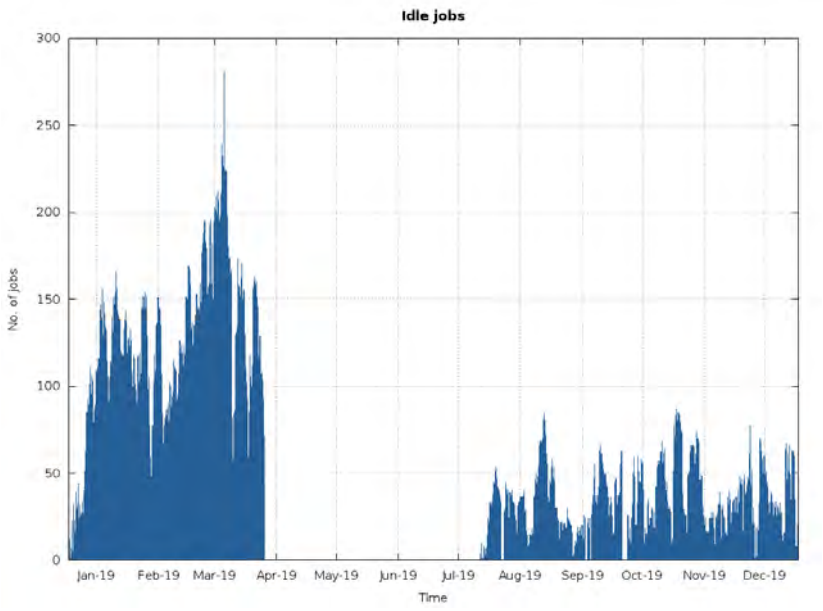
Active jobs, idle jobs & system backlog

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 the resources requested. The effect of the 105 day log maintenance is seen in both the GNU plots.

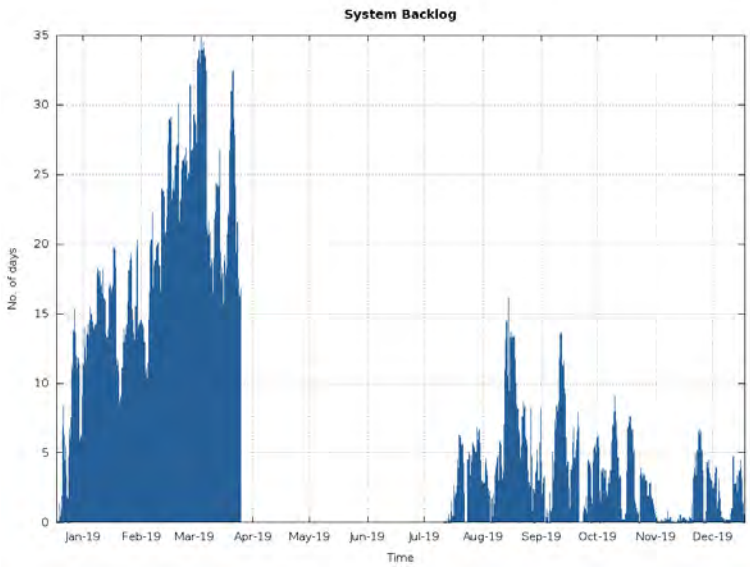
Active jobs



Idle jobs



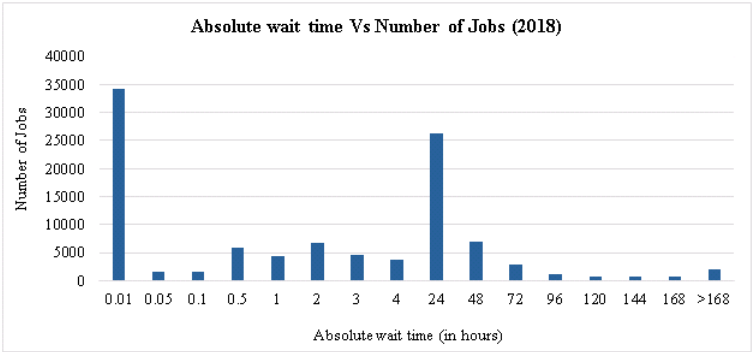
System backlog



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. The system backlog has reduced after the system unavailability due to decrease in number of jobs coming in, as there was no input and output data available after system was restored back to operation.

Absolute waittime Vs no. of jobs

Absolute wait time for a job is the time spent in the queue, after submission, till allocation of resources and execution. Above presentation is irrespective of job size. In 2019, 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 2019, more than 67% of the jobs have spent less than 1 day in queue.



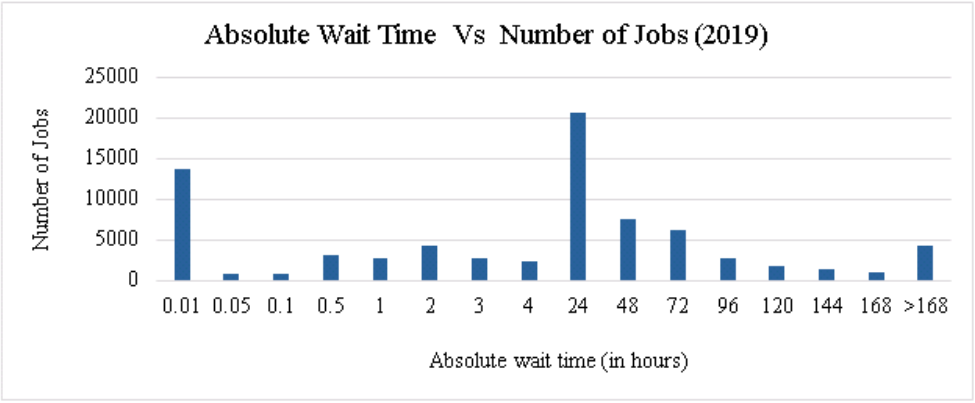
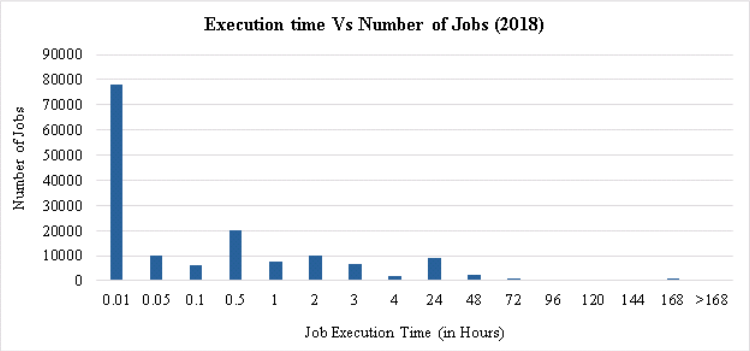


Table: Absolute waittime Vs no. of jobs

	No. of jobs	
Absolute wait time (in hours)	**Number of Jobs(2018)**	**Number of Jobs(2019)**
0.01	34243	13704
0.05	1641	832
0.1	1528	779
0.5	5826	3171
1	4348	2837
2	6836	4274
3	4610	2739
4	3836	2455
24	26366	20578
48	7017	7574
72	2915	6152
96	1051	2687
120	823	1854
144	722	1456
168	642	1073
>168	1942	4273

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



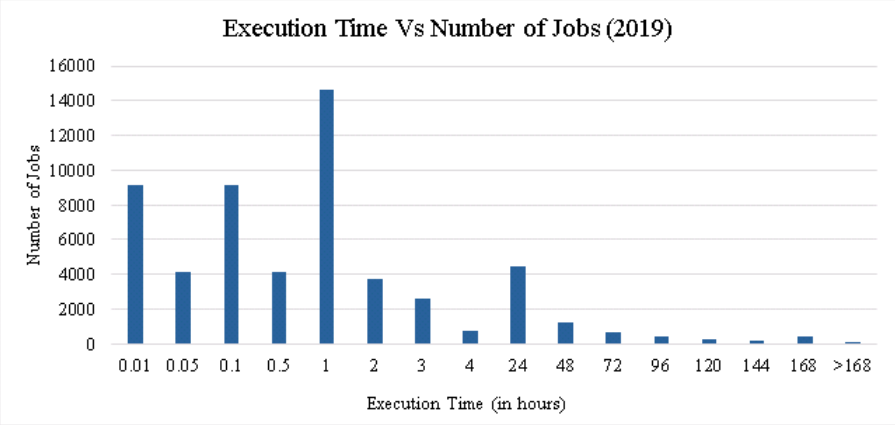


Table: Execution Time Vs Number of Jobs

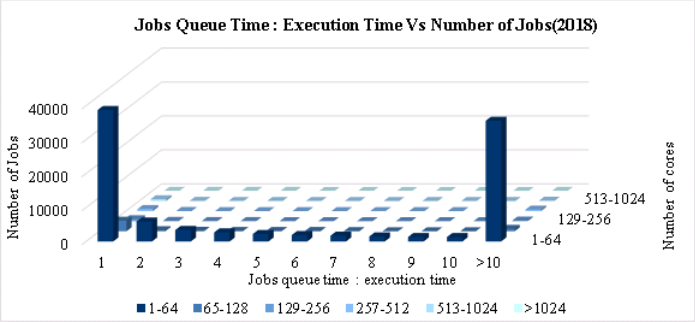
	Number of Jobs	
Execution Time (in hours)	**Number of Jobs (2018)**	**Number of Jobs (2019)**
0.01	78050	9155
0.05	10208	4143
0.1	6328	9155
0.5	20294	4143
1	7435	14657
2	9833	3745
3	6876	2577
4	2110	742
24	8918	4477
48	2167	1244
72	1125	680
96	654	402
120	562	228
144	383	209
168	1017	441
>168	65	115

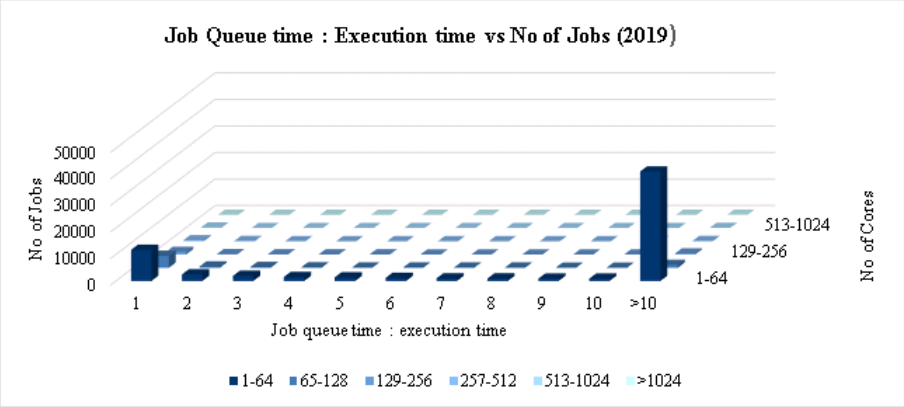
Above graph represents execution time of the jobs in hours. It is seen that only 0.74% of the total jobs executed for 7 days which is the maximum limit of the wall time of the jobs as compared to only 1% of the total jobs executed for 7 days last year.

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.





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.

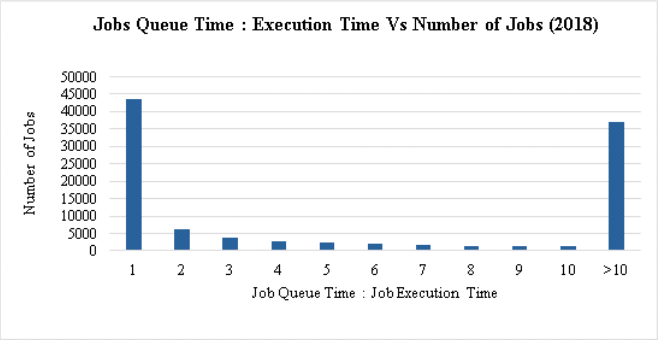
This segregation is made because job count for 1 to 64 CPU cores, being very high, diminishes bars for other job sizes, thus making observable distance between them nondescript.

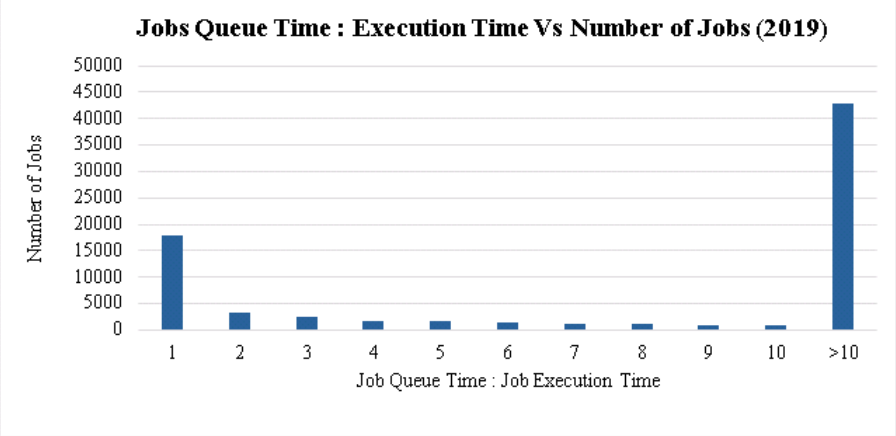
Table : Ratio of job waittime : execution time Vs number of jobs

2018	1	2	3	4	5	6	7	8	9	10	>10
1-64	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

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

2019	1	2	3	4	5	6	7	8	9	10	>10
1-64	11785	2525	1953	1541	1407	1166	1007	957	898	927	41257
65-128	4497	469	271	181	125	111	85	66	41	38	1073
129-256	968	145	88	44	42	28	22	22	17	10	388
257-512	377	106	31	10	11	11	6	5	4	2	81
513-1024	171	24	12	2	0	1	2	3	1	0	84
>1024	2	1	1	0	0	0	0	0	0	0	37

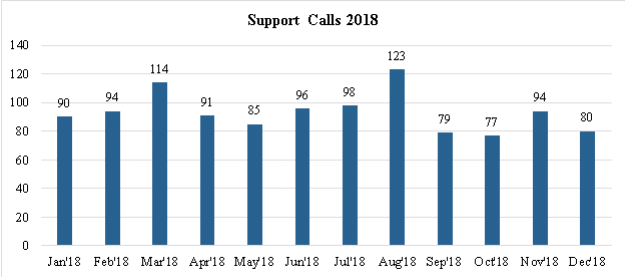




It can be seen from the graph that only 24% of the jobs have spent less than or equal amount of time in the queue as of its execution time (irrespective of job sizes). The percentage of turnaround time of the jobs has decreased by 8%, as compared to last year.

User support calls

Below Bar Graph shows the monthly wise distribution of support calls raised by users throughout the Year 2019. It can be seen that after Mar-2019 there was a sharp dip in the number of call raised it was due the unavailability of the system during that period.



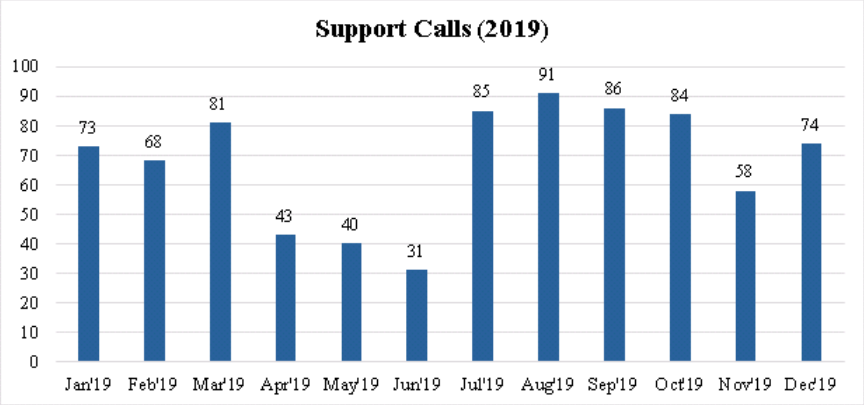


Table : Number of support calls

	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
2018	90	94	114	91	85	96	98	123	79	77	94	80
2019	73	68	81	43	40	31	85	91	86	84	58	74

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State wise CPU time utilization in %

NPSF user community is geographically distributed across 21 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 maximum number of users from Maharashtra.

Table: State wise CPU time utilization in %

State or Union Territory	Short Name	CPU Time	% CPU Time
Andhra Pradesh	AP	0	0
Arunachal Pradesh	AR	0	0
Assam	AS	194420531	0.144124102
Bihar	BR	145360800	0.107756082
Chandigarh	CH	5383295120	3.990641166
Chattisgarh	CG	0	0
National Capital Territory of Delhi	DL	1963870475	1.455818822
Goa	GA	0	0
Gujarat	GJ	5774818947	4.280878011
Haryana	HR	2386047947	1.768779335
Himanchal Pradesh	HP	3161035475	2.343278236
Jammu and Kashmir	J&K	0	0
Jharkhand	JK	104204584	0.077246945
Karnataka	KA	8609047840	6.38189435
Kerala	KL	128	9.48865E-08
Ladakh	LD	0	0
Madhya Pradesh	MP	3821817213	2.83311629
Maharashtra	MH	72380662107	53.65584524
Manipur	MN	1958490	0.00145183
Meghalaya	ML	0	0
Mizoram	MZ	0	0
Nagaland	NL	0	0
Odisha	OD	512155061	0.379660974
Pondicherry	PY	169917685	0.125960122
Punjab	PB	21664011854	16.05955007
Rajasthan	RJ	881079693	0.653145112
Sikkim	SK	0	0
Tamil Nadu	TN	42927294	0.031822039
Telangana	TS	362673496	0.268850165
Tripura	TR	0	0
Uttar Pradesh	UP	7170094230	5.315196838
Uttarakhand	UK	0	0
West Bengal	WB	168410431	0.124842793

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CPU Time Utilization in %

Disclaimer: The map depicted above is only a pictorial representation of INDIA and it's states, and is neither drawnto 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	% Job Count
Andhra Pradesh	AP	0	0
Arunachal Pradesh	AR	0	0
Assam	AS	185	0.226724022
Bihar	BR	67	0.082110862
Chandigarh	CH	624	0.764733998
Chattisgarh	CG	0	0
National Capital Territory of Delhi	DL	672	0.82355969
Goa	GA	0	0
Gujarat	GJ	1050	1.28558648
Haryana	HR	377	0.46202679
Himanchal Pradesh	HP	1706	2.090763141
Jammu and Kashmir	J&K	0	0
Jharkhand	JK	5	0.006127676
Karnataka	KA	186	0.227949557
Kerala	KL	2	0.002451071
Ladakh	LD	0	0
Madhya Pradesh	MP	1636	2.004975673
Maharashtra	MH	17125	20.9872912
Manipur	MN	65	0.079659791
Meghalaya	ML	0	0
Mizoram	MZ	0	0
Nagaland	NL	0	0
Odisha	OD	219	0.26839222
Pondicherry	PY	77	0.094366214
Punjab	PB	55131	67.56498401
Rajasthan	RJ	317	0.388494675
Sikkim	SK	0	0
Tamil Nadu	TN	361	0.442418226
Telangana	TS	510	0.625022979
Tripura	TR	0	0
Uttar Pradesh	UP	690	0.845619324
Uttarakhand	UK	0	0
West Bengal	WB	590	0.725516869

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Jobs Processed

Jobs Processed in %

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

Table: State wise projects

State or Union Territory	Short Name	Number of Active Projects
Andhra Pradesh	AP	0
Arunachal Pradesh	AR	0
Assam	AS	18
Bihar	BR	4
Chandigarh	CH	8
Chattisgarh	CG	0
National Capital Territory of Delhi	DL	16
Goa	GA	1
Gujarat	GJ	18
Haryana	HR	6
Himanchal Pradesh	HP	9
Jammu and Kashmir	J&K	0
Jharkhand	JK	2
Karnataka	KA	27
Kerala	KL	4
Ladakh	LD	0
Madhya Pradesh	MP	5
Maharashtra	MH	164
Manipur	MN	2
Meghalaya	ML	0
Mizoram	MZ	1
Nagaland	NL	0
Odisha	OD	9
Pondicherry	PY	2
Punjab	PB	18
Rajasthan	RJ	15
Sikkim	SK	0
Tamil Nadu	TN	10
Telangana	TS	24
Tripura	TR	0
Uttar Pradesh	UP	18
Uttarakhand	UK	3
West Bengal	WB	14

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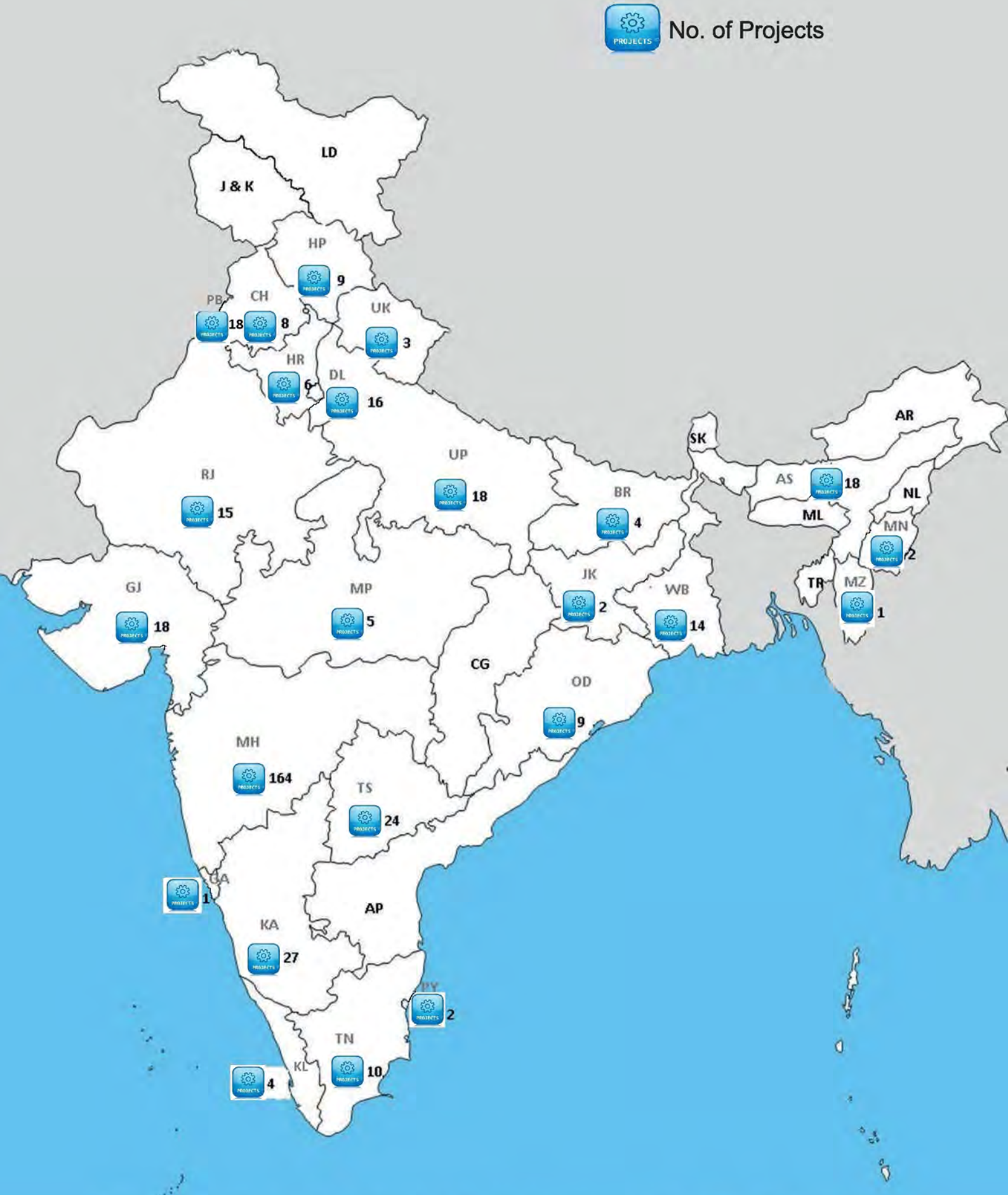
Projects



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

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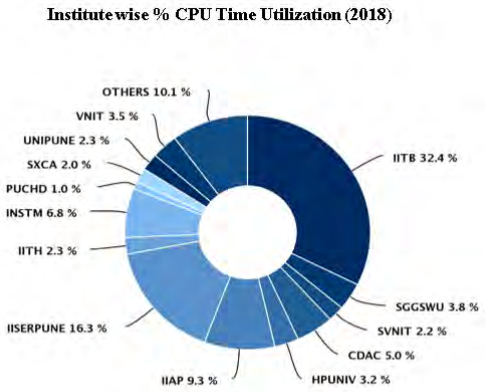
4.2 Users and Institutes

Institute wise CPU time utilization

User2s Jobs running over the cluster consumes CPU Time of the cluster. Below doughnut plot represents the % distribution of CPU Time consumed by the Research Organizations/Academic Institutes. As seen in the 2018 and 2019 plots, Jobs submitted from users of IIT Bombay is continuously consuming the max. % of CPU Time.



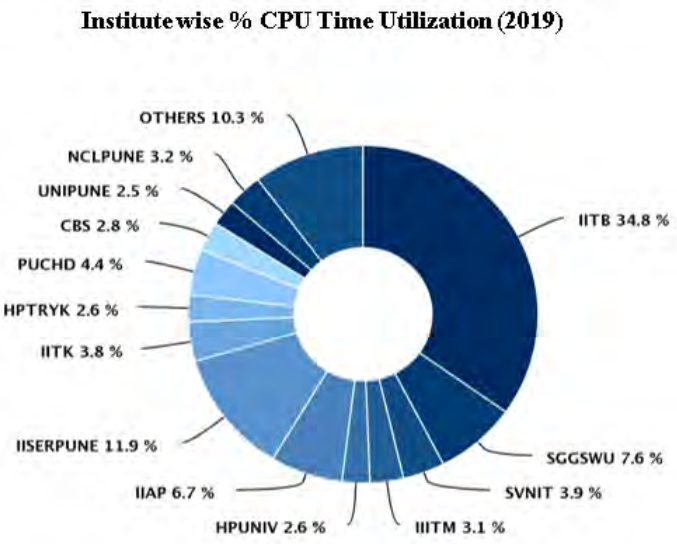


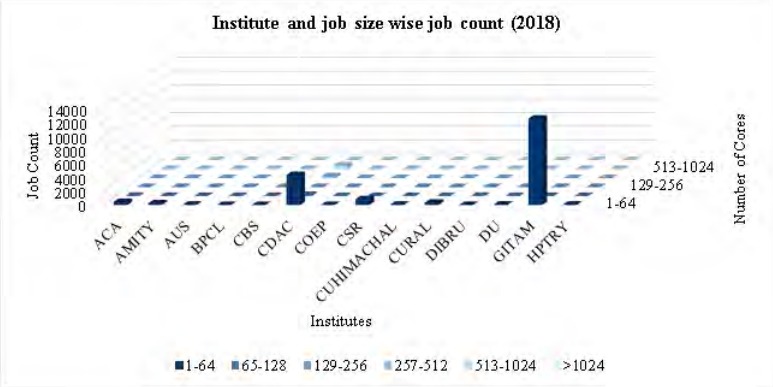
Table : Institute wise %CPU time utilization Year-2018

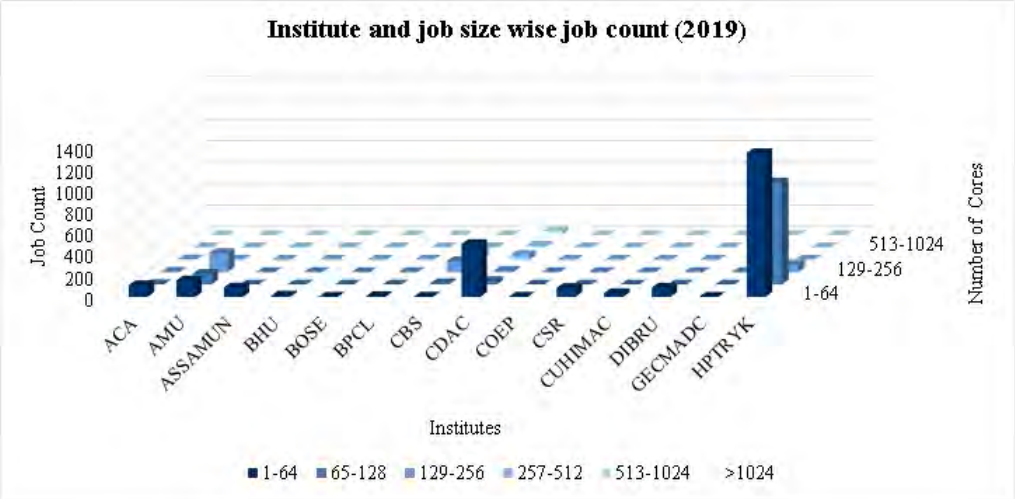
Institute	CPU Time Utilization(seconds)
IITB	46090269566
SGGSWU	5344430440
SVNIT	3067733056
CDAC	7061825270
HPUNIV	4570447664
IIAP	13195440637
IISERPUNE	23221259633
IITH	3262155957
INSTM	9656791940
PUCHD	1439861225
SXCA	2856237025
UNIPUNE	3312310994
VNIT	4925276370
OTHERS	14397019008

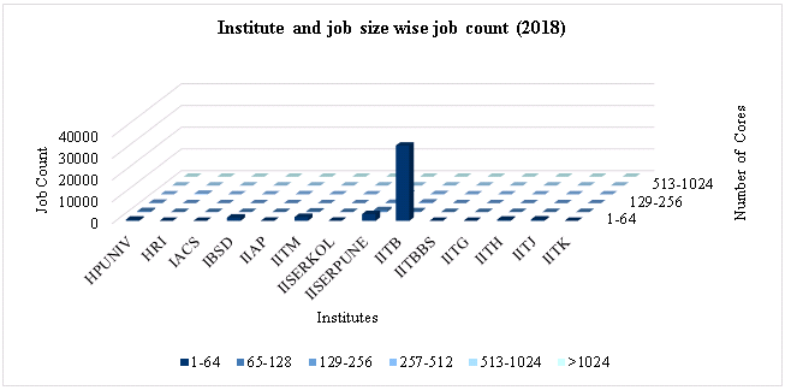
Table : Institute wise %CPU time utilization Year-2019

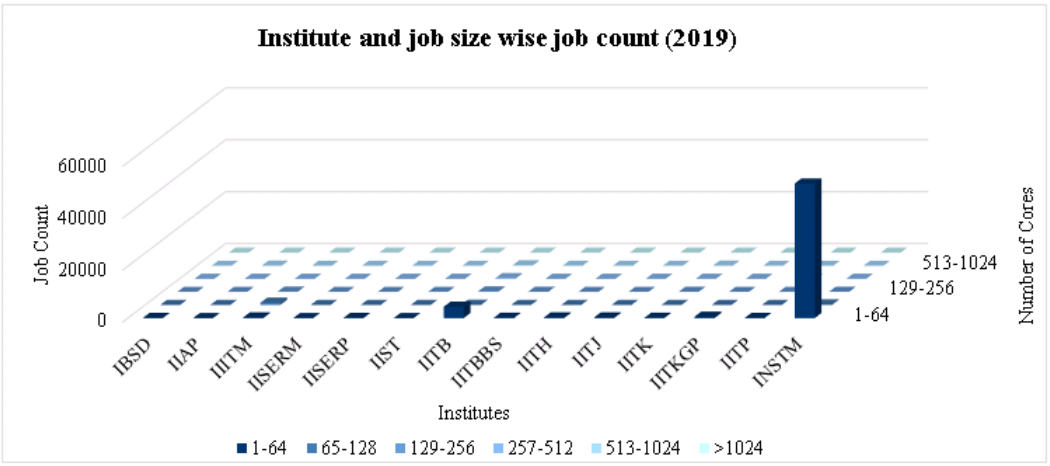
Institute	CPU Time Utilization(seconds)
IITB	42850701633
IISERP	14594041136
SGGSWU	9317473024
IIAP	8249226240
PUCHD	5383295120
SVNIT	4760117152
IITK	4622852034
NCLPUNE	3946017617
IIITM	3818456813
CBS	3446545744
HPTRYK	3193726574
HPUNIV	3146808947
UNIPUNE	3034532016
OTHERS	12647639197

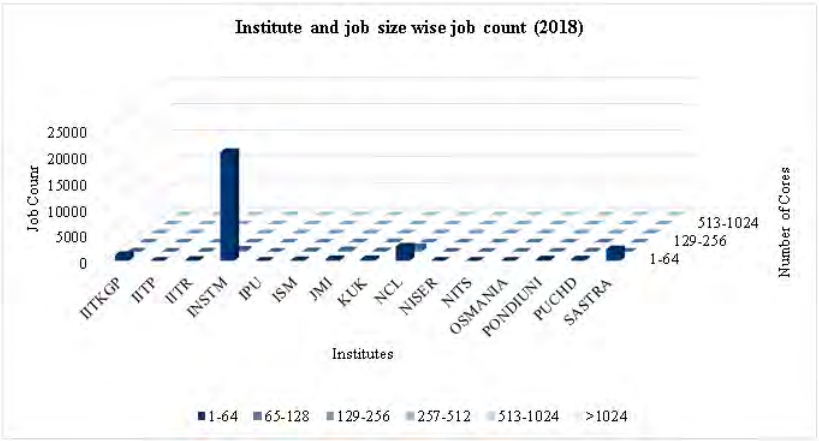
Institute and job size wise job count

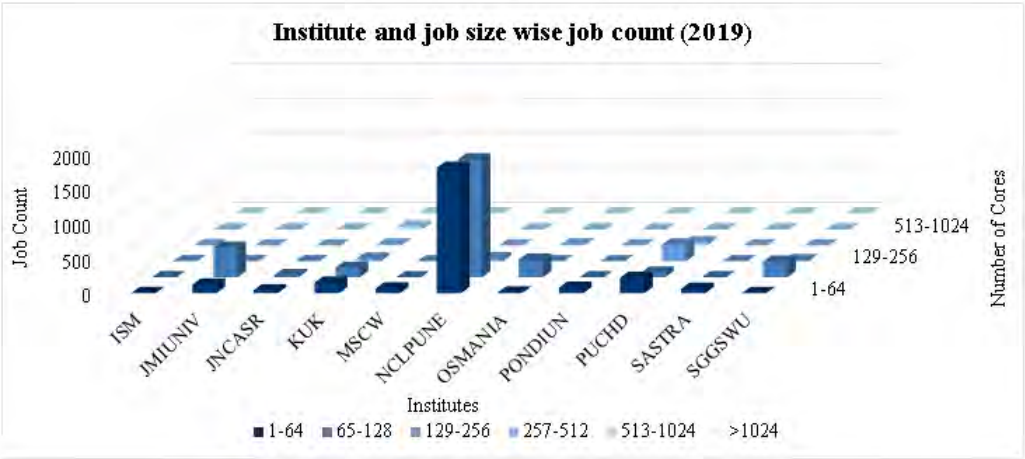


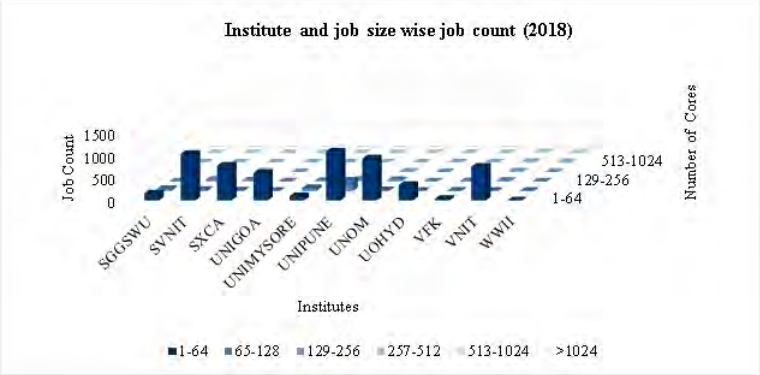



Institute and job size wise job count (2018)
Job Count
40000
30000
20000
10000
0
IIPUNIV
HRI
IACS
IBSD
IIAP
IITM
IISERKOL
IISERPUNE
IITB
IITBBS
IITG
IITH
IITJ
IITK
Institutes
513-1024
129-256
1-64
Number of Cores
1-64
65-128
129-256
257-512
513-1024
>1024


Institute and job size wise job count (2019)
Job Count
60000
40000
20000
0
IBSD
IIAP
IIITM
IISERM
IISERP
IIST
IITB
IITBBS
IITH
IITJ
IITK
IITKGP
IITP
INSTM
Institutes
513-1024
129-256
1-64
Number of Cores
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
Institutes
513-1024
129-256
1-64
Number of Cores
1-64
65-128
129-256
257-512
513-1024
>1024


Institute and job size wise job count (2019)
Job Count
2000
1500
1000
500
0
ISM
JMIUNIV
JNCASR
KUK
MSCW
NCLPUNE
OSMANIA
PONDIUN
PUCHD
SASTRA
SGGSWU
Institutes
513-1024
129-256
1-64
Number of Cores
1-64
65-128
129-256
257-512
513-1024
>1024



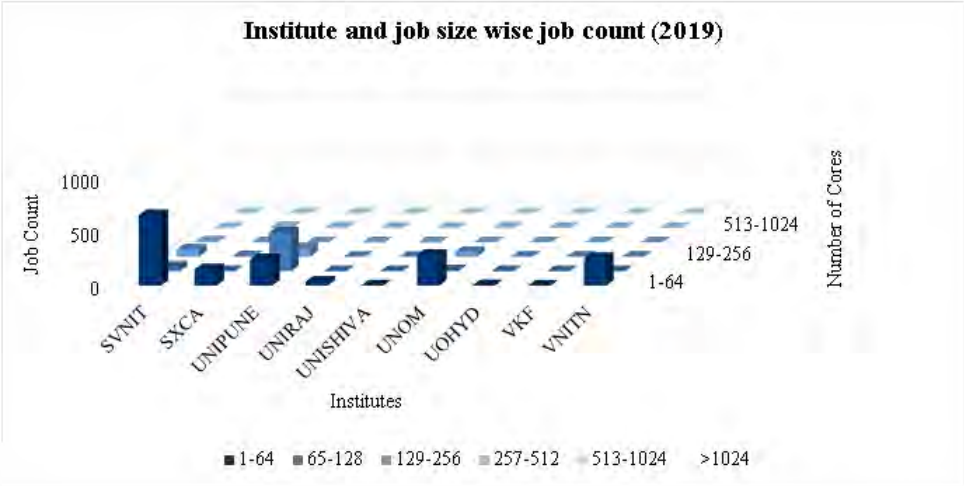


Table: Institute and Job size wise Job count Year - 2018

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
HPI	547	431	170	8	0	0

Continued on next page

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Institute	1-64	65-128	129-256	257-512	513-1024	>1024
IACS	7	1	0	300	0	0
IBSD	1	7	0	0	0	0
IIAP	1535	29	2	3	0	0
IIITM	16	27	4	56	38	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	0	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	0	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	0	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
UNIGOA	567	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

Table: Institute and Job size wise Job count Year - 2019

Institute	1-64	65-128	129-256	257-512	513-1024	>1024
ACA	109	3	2	5	0	0
AMU	153	99	177	2	0	0
ASSAMUNIV	88	0	0	0	0	0
BHU	12	0	0	0	0	0
BOSE	1	0	0	0	0	0
BPCL	8	0	0	0	0	0
CBS	2	11	101	83	0	0
CDAC	493	31	14	44	15	36
COEP	2	0	0	0	0	0
CSR	82	0	0	0	0	0
CUHIMACHALS	36	0	0	0	0	0
DIBRU	86	3	0	0	0	0
GECMADOSA	1	0	0	0	0	0
HPTRYK	1342	952	67	2	0	0
HPUNIV	583	641	277	35	21	0
IBSD	65	0	0	0	0	0
IIAP	0	0	0	0	25	2
IIITM	254	861	132	0	0	0
IISERB	4	0	0	0	0	0
IISERM	45	1	1	0	0	0
IISERP	479	778	164	56	0	0
IIST	2	0	0	0	0	0
IITB	4357	66	208	254	150	20
IITBBS	148	12	50	1	0	0
IITH	223	0	0	0	0	0
IITJ	267	0	0	0	0	0
IITK	90	15	21	43	34	0
IITKGP	501	18	0	0	0	0
IITP	65	2	0	0	0	0
INSTM	51844	230	72	36	2	1
ISM	1	1	0	2	0	0
JMIUNIV	123	424	1	0	0	0
JNCASR	39	30	0	0	0	0
KUK	152	134	38	13	42	0
MSCW	67	0	0	0	0	0
NCLPUNE	1803	1693	45	0	0	0
OSMANIA	11	254	0	12	0	0
PONDIUNI	77	0	0	0	0	0
PUCHD	221	65	239	47	0	1

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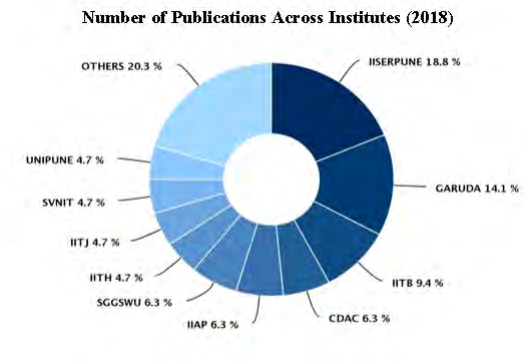
Institute	1-64	65-128	129-256	257-512	513-1024	>1024
SASTRA	62	0	0	0	0	0
SGGSWU	2	223	15	0	0	0
SVNIT	660	40	68	8	0	0
SXCA	152	1	3	0	6	0
UNIPUNE	247	362	79	1	3	0
UNIRAJ	37	0	0	0	0	0
UNISHIVAJI	2	0	0	0	0	0
UNOM	289	8	0	0	2	0
UOHYD	3	0	0	0	0	0
VKF	1	0	0	0	0	0
VNITN	257	0	0	0	0	0

Number of publications across institutes

User2s Research work resulted to Publications, below doughnut plot represents the % wise publications across Research Organizations/Academic Institutes. In Year 2019 total 52 Publications has been published using PARAM Yuva II cluster.



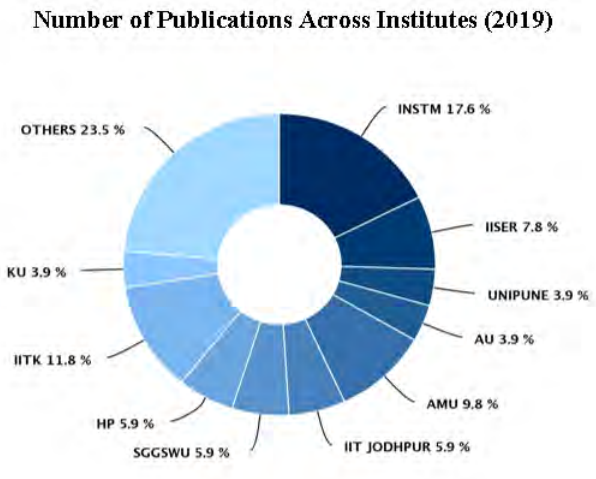


Table: Number of publications across institutes Year - 2018

Institute	Number of Publications
IISERPUNE	12
GARUDA	9
IITB	6
CDAC	4
IIAP	4
SGGSWU	4
IITH	3
IITJ	3

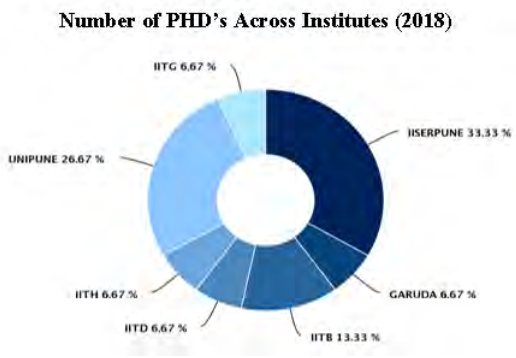
SVNIT	3
UNIPUNE	3
BASPONC	2
INSTM	2
IIITM	1
IISC	1
IISERTVM	1
IITKVP	1
IITG	1
NISER	1
PONDIUM	1
SASTRA	1

Table: Number of publications across institutes Year-2019

Institute	**Number of Publications**
INST Mohali	9
IISER	4
IIAP-Indian Institute of AstroPhysics	1
Unipune-Pune University	2
AssamUniv	2
AMU-Aligarh Muslim University	5
IIT Guwhati	1
NCL Pune	1
IIT Jodhpur	3
SGGSWU	3
IPU- Indra Prasth University	1
HP university	3
IIT Kanpur	6
CBS Mumbai	1
Osmania Hyderabad	1
dibru- Dibrugarh University	1
GEC Madosa	1
JamiaUniv-Jamia Milia University	2
Kurukshetra University	3
Punjab University	2

Number of Ph.D's across institutes

In Year 2019, four of the PARAM Yuva II Users has completed Ph.D. and submitted the thesis, below are the details.



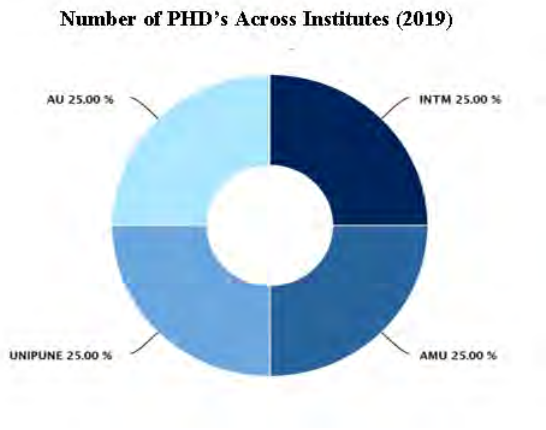


Table: Number of Ph.D's across institutes Year - 2018

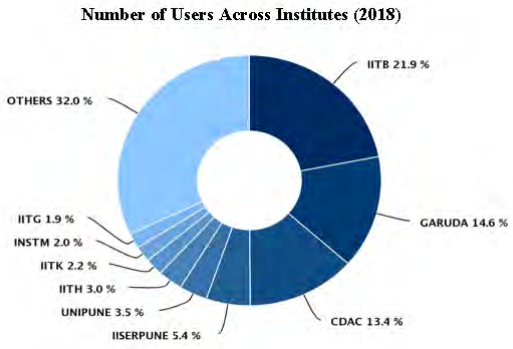
Institute	Number of Ph.D's
IISERPUNE	5
GARUDA	1
IITB	2
IITD	1
IITH	1
UNIPUNE	4
IITG	1

Table: Number of Ph.D's across institutes Year - 2019

Institute	Number of Ph.D's
INSTM	1
AMU	1
UNIPUNE	1
ASSAMUNIV	1

Number of Users across institutes

In Year 2019, 63 Users and 8 Institutes has been registered to PARAM Yuva II resulted to total user count of 1193. Below plots is the % distribution of the users among the Institutes.



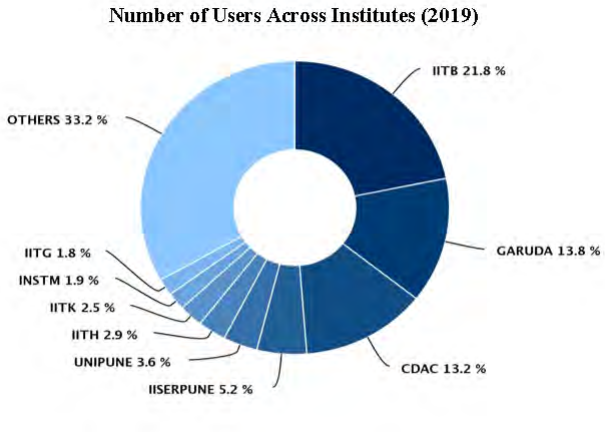


Table: Number of users across institutes Year - 2018

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

Table: Number of users across institutes Year - 2019

Institute	**Number of Users**
IITB	260
GARUDA	165
CDAC	157
IISERPUNE	62
UNIPUNE	43
IITH	34
IITK	30
INSTM	23
IITG	22
OTHERS	396

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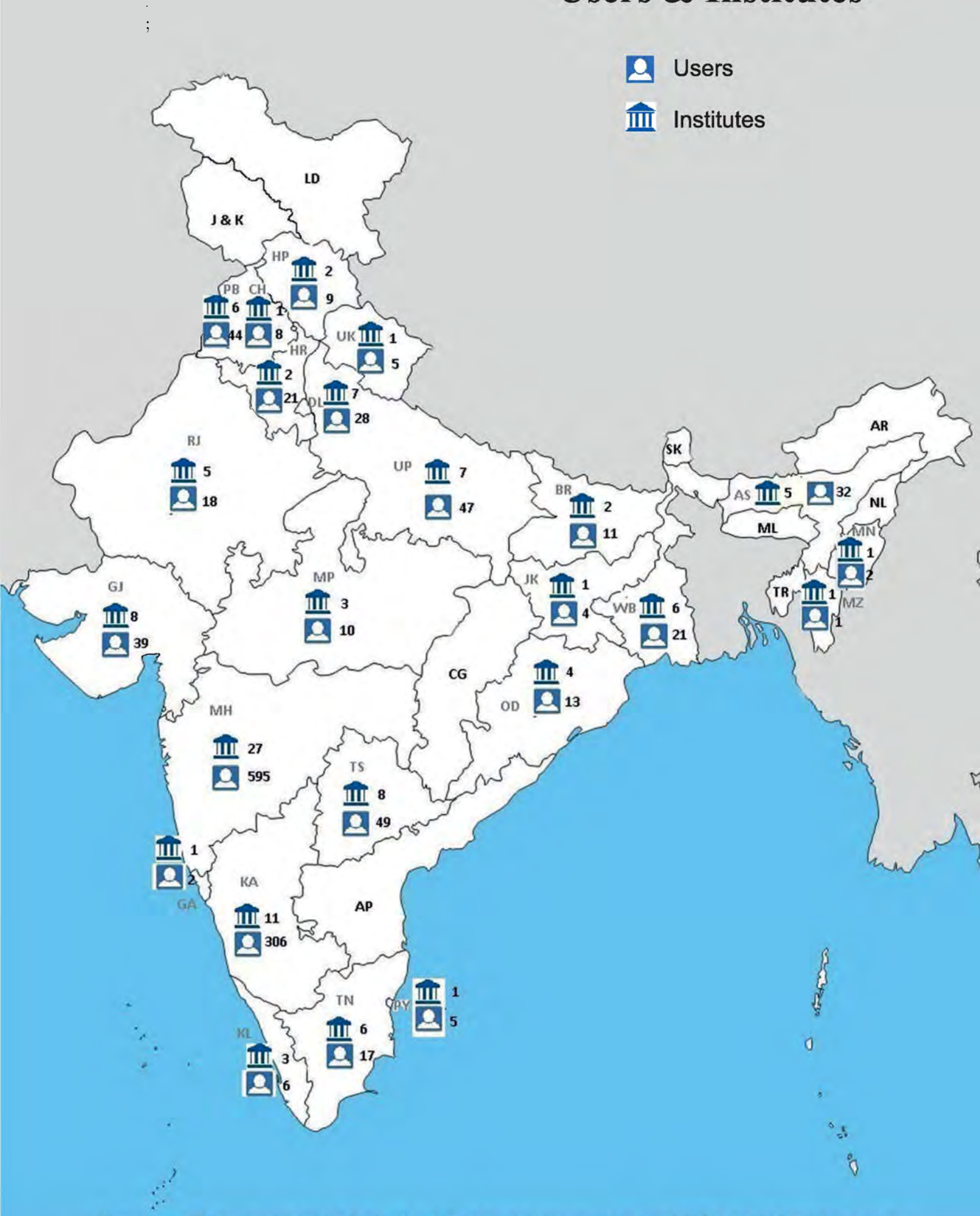
Table: State wise NPSF Users and Institutes

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	11
Chandigarh	CH	1	8
Chattisgarh	CG	0	0
National Capital Territory of Delhi	DL	7	28
Goa	GA	1	2
Gujarat	GJ	8	39
Haryana	HR	2	21
Himanchal Pradesh	HP	2	9
Jammu and Kashmir	J&K	0	0
Jharkhand	JK	1	4
Karnataka	KA	11	306
Kerala	KL	3	6
Ladakh	LD	0	0
Madhya Pradesh	MP	3	10
Maharashtra	MH	27	595
Manipur	MN	1	2
Meghalaya	ML	0	0
Mizoram	MZ	1	1
Nagaland	NL	0	0
Odisha	OD	4	13
Pondicherry	PY	1	5
Punjab	PB	6	44
Rajasthan	RJ	5	18
Sikkim	SK	0	0
Tamil Nadu	TN	6	17
Telangana	TS	8	49
Tripura	TR	0	0
Uttar Pradesh	UP	7	47
Uttarakhand	UK	1	5
West Bengal	WB	6	21

Users & Institutes



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

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4.3 Research Field

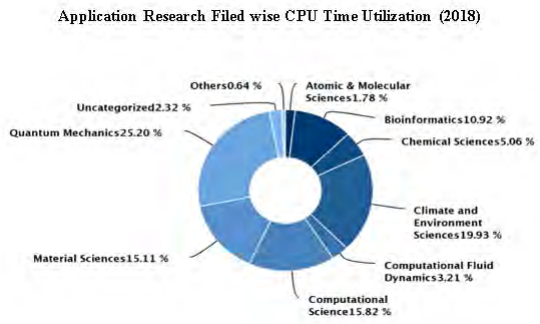
User's when affiliated with NPSF are classified according to their 1) Research Field, and 2) Institute. Former is deduced from area of work/application, whereas Institute is one of the attribute in Technical Affiliation Scheme (TAS) form. In this section, we have presented CPU time distribution, job 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.

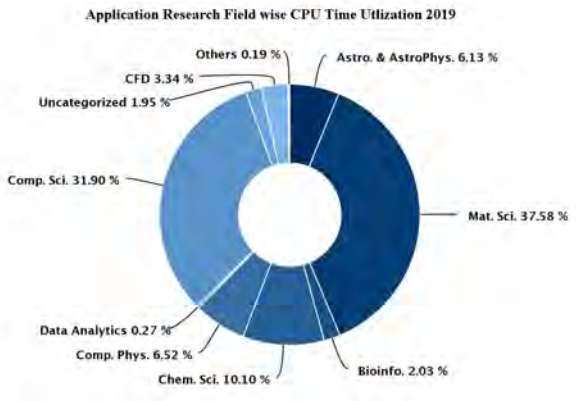
Table : List of application research fields on NPSF

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

Below doughnut plot represents the % CPU Time utilization by the jobs across application research fields. Material Science and Computational Science are the major contributors towards the CPU time utilization and the Jobs count.



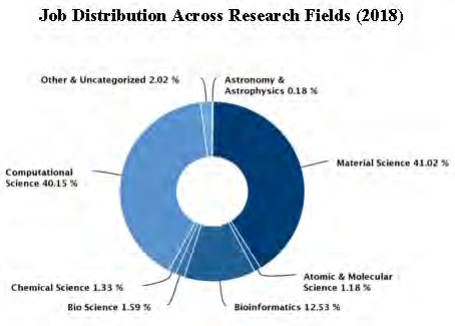


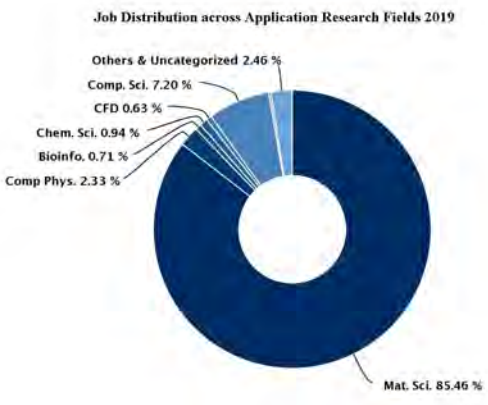
Above plots brings forth CPU time distribution across various application research fields.

Table: Research Field wise CPU time utilization

	CPU time in seconds	
Application Research Field	**2018**	**2019**
Astronomy and Astrophysics	0	8249226240
Atomic & Molecular Sciences	552104334	615
Bio Sciences	259768576	1958586
Bioinformatics	7297809945	2731660017
Chemical Sciences	284302966	13581185416
Climate and Environment Sciences	5473111638	379182337
Complex Systems and Statistical Physics	0	0
Computational Fluid Dynamics	154974099	4489924639
Computational Physics	0	8768951681
Computational Sciences	301228639	42908478613
Data analytics	1144878	362913144
Geological Sciences	3037660	104204584
Material Science	6051030366	50551931751
Quantum Mechanics	1596156672	145360928
Structural Mechanics	19760	0
Uncategorized	1938219316	2622816306

Job distribution across application research fields



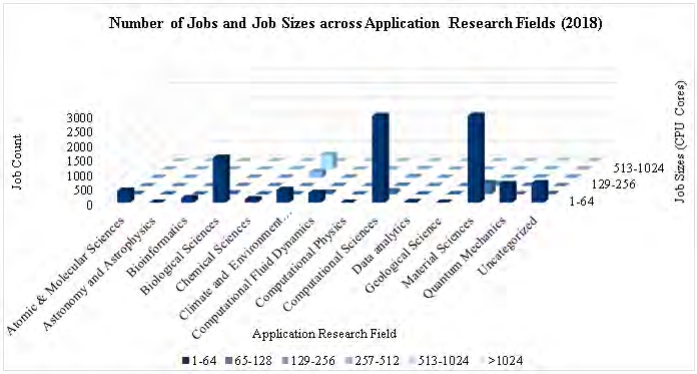


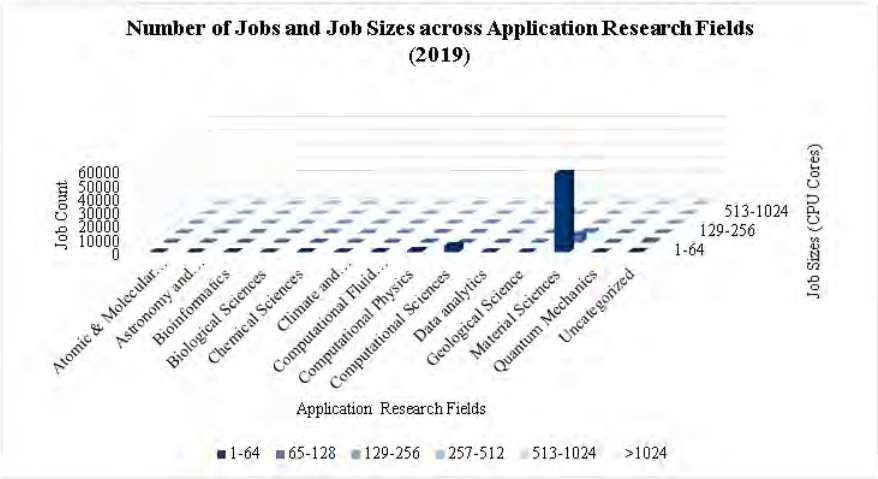
Above plots shows application research fields wise percentage distribution of number of jobs processed.

Table:Job distribution across application research fields

	No. of Jobs	
Application Research Field	**Job Count 2018**	**Job Count 2019**
Atomic & Molecular Sciences	1192	10
Astronomy and Astrophysics	182	27
Bioinformatics	12751	537
Biological Sciences	1620	67
Chemical Science	1359	706
Climate and Environment Sciences	1191	143
Computational Fluid Dynamics	398	473
Complex systems & statistical physics	99	0
Computational Physics	5	1752
Computational Science	40871	5417
Data analytics	19	207
Geological Science	6	4
Material Science	41761	64340
Quantum Mechanics	690	69
Uncategorized	2061	1532

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 (2018)

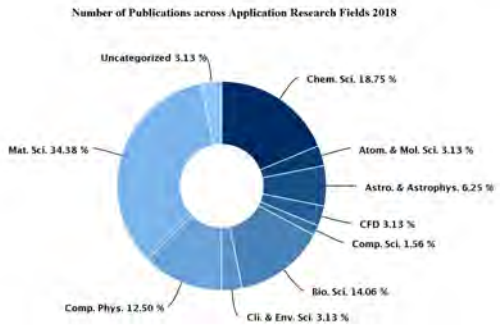
Application Research Fields	**1-64**	**65-128**	**129-256**	**257-512**	**513-1024**	**>1024**
Atomic & Molecular Sciences	407	14	0	0	0	0
Astronomy and Astrophysics	0	0	0	0	0	0
Bioinformatics	152	0	0	0	0	0
Biological Sciences	1535	29	2	3	0	0
Chemical Sciences	117	0	0	6	16	0
Climate and Environment Sciences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

Table: Number of Jobs and Job Sizes across Application Research Fields 2019

Application Research Fields	**1-64**	**65-128**	**129-256**	**257-512**	**513-1024**	**>1024**
Atomic & Molecular Sciences	10	0	0	0	0	0
Astronomy and Astrophysics	0	0	0	0	25	0
Bioinformatics	212	101	177	8	6	33
Biological Sciences	67	0	0	0	0	0
Chemical Sciences	273	3	0	83	0	0
Climate and Environment Sciences	102	3	0	38	0	0
Computational Fluid Dynamics	360	15	21	43	34	0
Computational Physics	1173	199	277	60	42	1
Computational Sciences	4709	74	208	254	152	20
Data analytics	152	29	14	0	9	3
Geological Science	1	1	0	2	0	0
Material Sciences	57941	5308	908	150	32	1
Quantum Mechanics	67	2	0	0	0	0
Uncategorized	481	992	53	6	0	0

Number of publications across research fields

Below doughnut plot represents the % number of Publications across Application Research field. Majority of the Publications belongs to Material Science domain.



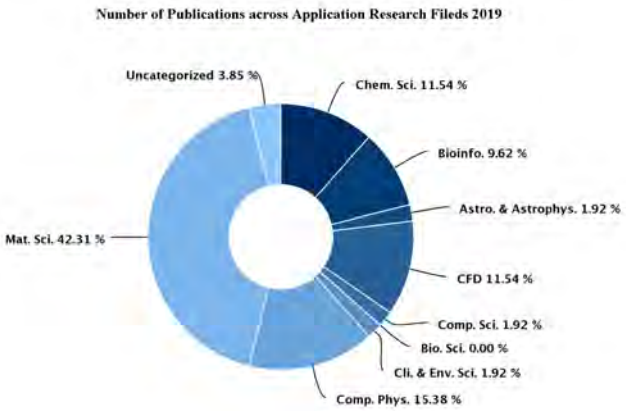
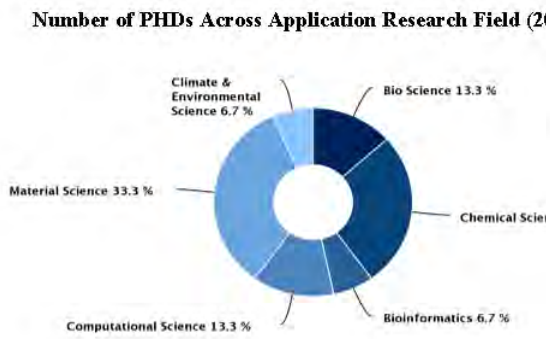


Table: Number of publications across research fields

	Number of publicatons	
Application Research Fields	**Publication Count 2018**	**Publication Count 2019**
Astronomy & Astrophysics	4	1
Atomic and Molecular Science	2	0
Bioinformatics	0	5
Bio Science	9	0
Chemical Science	12	6
Climate & Environmental Science	2	1
Complex Systems & Statstical Physics	0	0
Computational Fluid Dynamics	2	6
Computational Physics	8	8
Computational Science	1	1
Geological Science	0	0
Material Science	22	22
Uncategorized	2	2

Number of PhDs across research fields



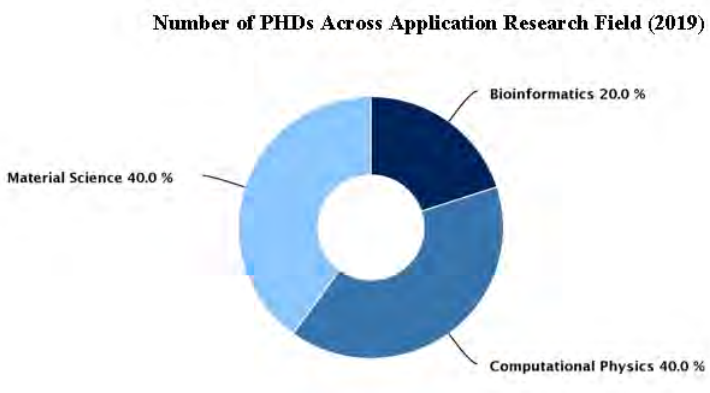
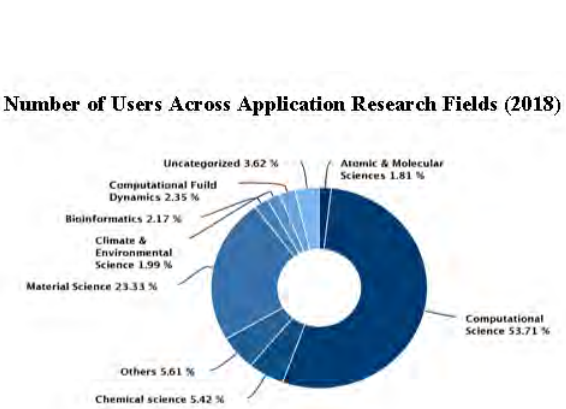


Table: Number of PhDs across research fields

	Number of PhDs	
Application Research Fields	**Number of PHDS 2018**	**Number of PHDS 2019**
Bio Science	2	0
Chemical Science	4	0
Bioinformatics	1	1
Computational Science	2	0
Material Science	5	2
Climate & Environmental Science	1	0
Computational Physics	0	1

Number of users across research fields

Below doughnut plot shows the % distribution of users among the research areas. Majority of the users belongs to Computational science and Material Science domains.



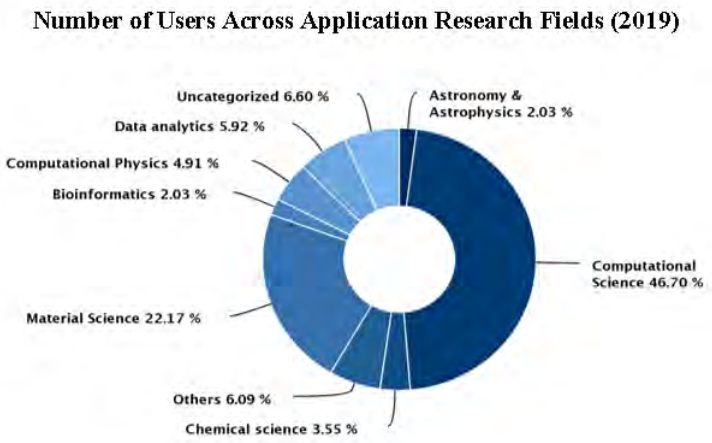


Table: Number of users across research fields

	Number of Users	
Application Research Fields	**Number of users 2018**	**Number of users 2019**
Astronomy & Astrophysics	3	12
Atomic & molecular Science	10	4
Bio Science	6	3
Bioinformatics	12	12
Chemical Science	30	21
Climate & Environmental Science	11	10
Complex System & Statistical Physics	1	0
Computational Fluid Dynamics	13	10
Computational Physics	1	29
Computational Science	297	276
Data Analytics	2	35
Geological Science	6	5
Material Science	129	131
Quantum Mechanics	2	4
Uncategorized	20	39

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Table: State wise Number of Publications and PhDs

State or Union Territory	**Short Name**	**No. of Publications**	**No. of PhDs**
Andhra Pradesh	AP	0	0
Arunachal Pradesh	AR	0	0
Assam	AS	4	1
Bihar	BR	0	0
Chandigarh	CH	0	0
Chattisgarh	CG	0	0
National Capital Territory of Delhi	DL	3	0
Goa	GA	0	0
Gujarat	GJ	1	0
Haryana	HR	0	0
Himanchal Pradesh	HP	3	0
Jammu and Kashmir	J&K	0	0
Jharkhand	JK	0	0
Karnataka	KA	1	0
Kerala	KL	0	0
Ladakh	LD	0	0
Madhya Pradesh	MP	0	0
Maharashtra	MH	8	1
Manipur	MN	0	0
Meghalaya	ML	0	0
Mizoram	MZ	0	0
Nagaland	NL	0	0
Odisha	OD	0	0
Pondicherry	PY	0	0
Punjab	PB	12	1
Rajasthan	RJ	3	0
Sikkim	SK	0	0
Tamil Nadu	TN	0	0
Telangana	TS	1	0
Tripura	TR	0	0
Uttar Pradesh	UP	11	1
Uttarakhand	UK	0	0
West Bengal	WB	0	0

;

Number of PhDs & Publications

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

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4.4 Queue

Job Submission Queues

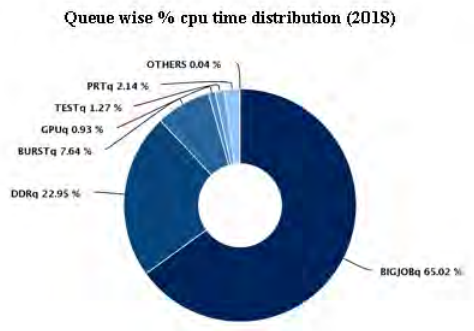
Various queues ensures a spectrum of quality of service according to the resource requirement of the users for different computing exercises. Below table shows the summary of job submission queues.

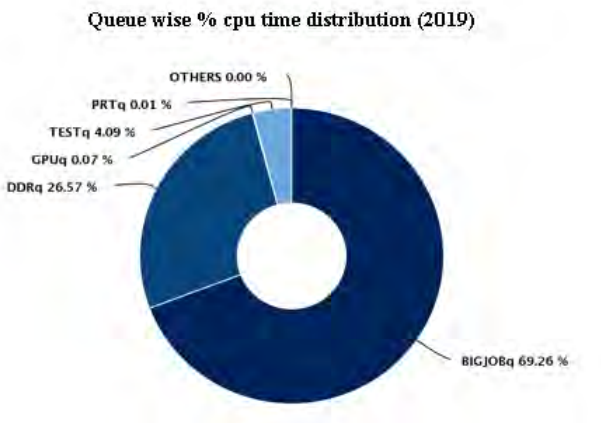
Table : Summary of queues on NPSF

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



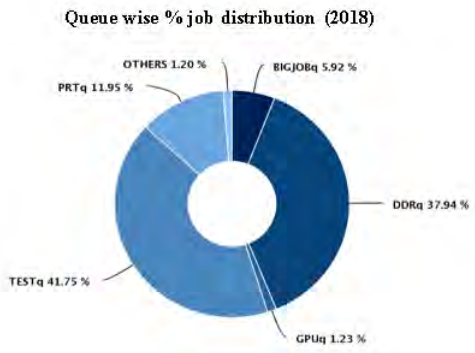


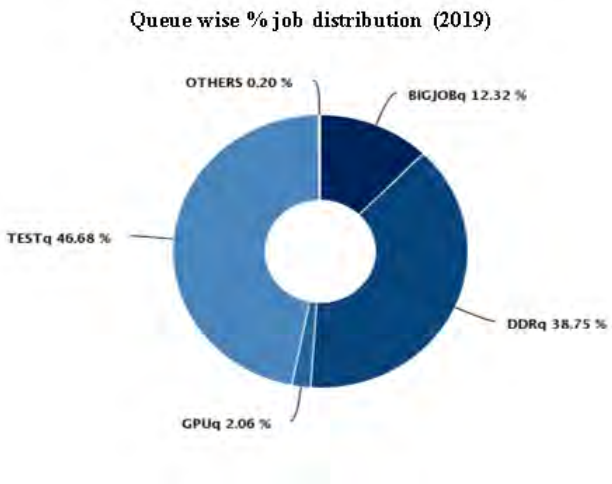
Above graph shows distribution in percentage of CPU time utilized by jobs in respective queues. As seen from the doughnut, there is lion2s share of cputime utilization by jobs routed through BIGJOBq i.e. jobs requiring more than 64 cores. This is indicator of more capability computing than capacity computing.

Table: Queue wise cpu time distribution

	CPU Time (Hours)	
Queue	**2018**	**2019**
BIGJOBq	25595859.52	2.28188E+11
BURSTq	3008839.749	30720
DDRq	9035466.181	87545553168
FDRq	960.808	5
GPUq	364162.744	222430320
PRTq	841979.58	25921056
SDSq	170208.331	2253184
TESTq	499686.026	13464444799
BENCHq	0	806284
DGXq	0	4506

Distribution of jobs w.r.t. queues



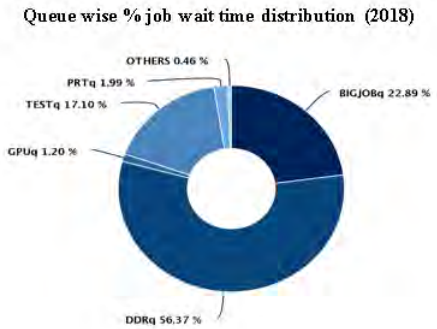


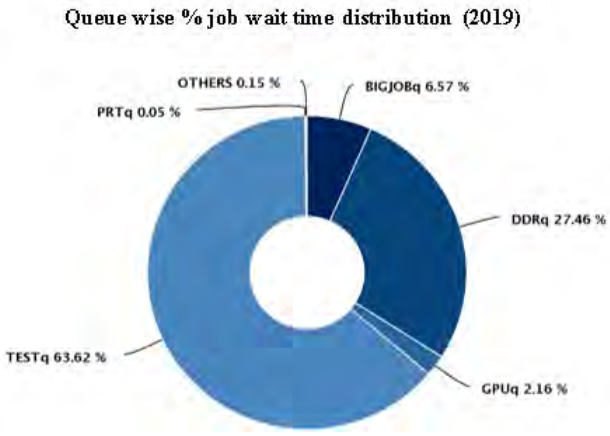
Above graph shows distribution in percentage of jobs among execution queues. It is seen from the graphs that there is 10% increase in the big jobs (jobs requiring more than 64 cores) than last year. This also compliments the argument of more capability computing than capacity computing.

Table: Queue wise jobs distribution

	Number of jobs	
Queue	**2018**	**2019**
BIGJOBq	6168	9255
BURSTq	921	6
DDRq	39541	29111
FDRq	204	4
GPUq	1287	1544
PRTq	12449	27
SDSq	129	28
TESTq	43512	35067
BENCHq	0	54
DGXq	0	33

Distribution of wait time w.r.t. queues



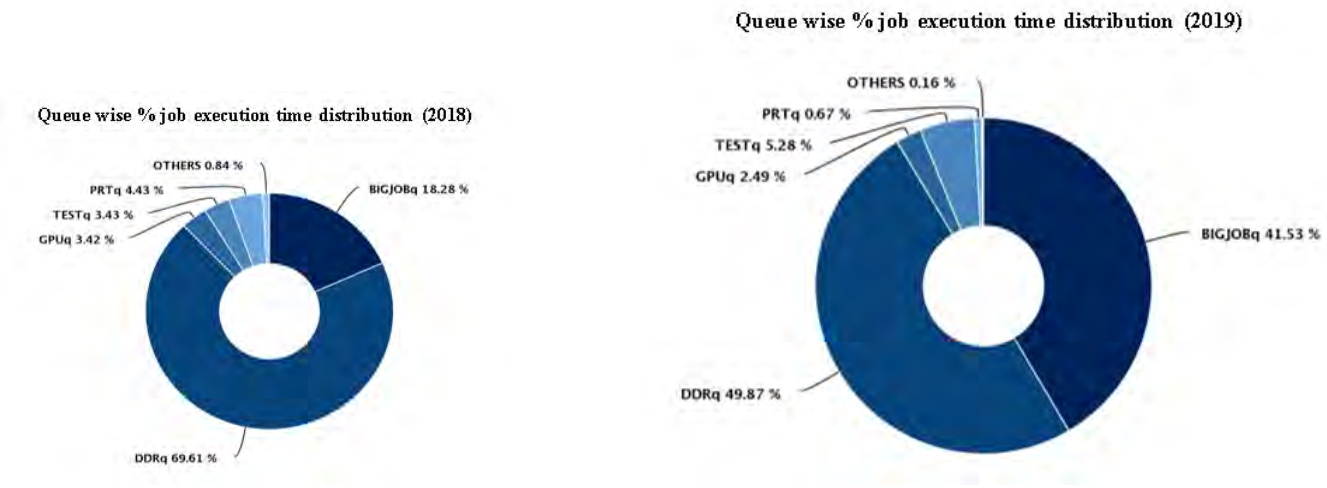


Above graph is a representation of percentage distribution of time spent by jobs, once submitted, until allowed for execution on system. The wait time of the jobs requesting for large resources is less than wait time of the jobs requiring less resources. This is due to the availability of more resources in BIGJOBq than in DDRq and TESTq.

Table: Queue wise Wait Time distribution

	Wait Time (Hours)	
Queue	**2018**	**2019**
BIGJOBq	430203.969	176570
BURSTq	7709.271	4017
DDRq	1059568.325	737873
FDRq	857.976	0
GPUq	22520.742	57927
PRTq	37444.241	1285
SDSq	69.779	9
TESTq	321400.491	1709663
BENCHq	0	49

Distribution of execution time w.r.t. queues

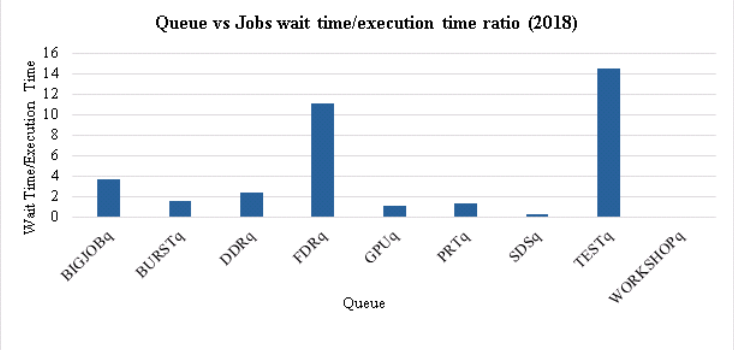


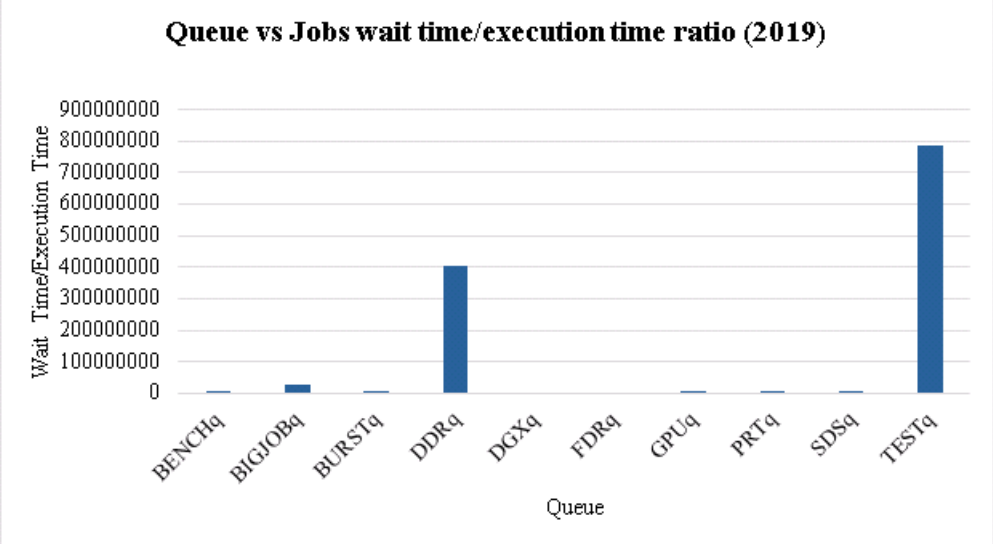
Above doughnuts shows % job execution time (time period for which job executes on the compute nodes) distributed across various queues. As compared to last year, the execution time of the BIG Jobs has increased by 23%.

Table: Queue wise job execution time distribution

	Execution Time (Hours)	
Queue	**2018**	**2019**
BIGJOBq	118777.135	141137
BURSTq	5020.644	10
DDRq	452364.064	169457
FDRq	77.911	1
GPUq	22231.962	8451
PRTq	28781.022	2269
SDSq	359.151	116
TESTq	22262.192	17953
BENCHq	0	412
DGXq	0	3

Queue vs Jobs wait time / execution time ratio



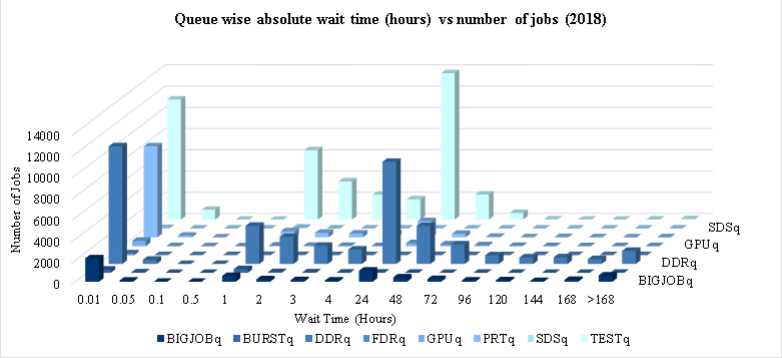


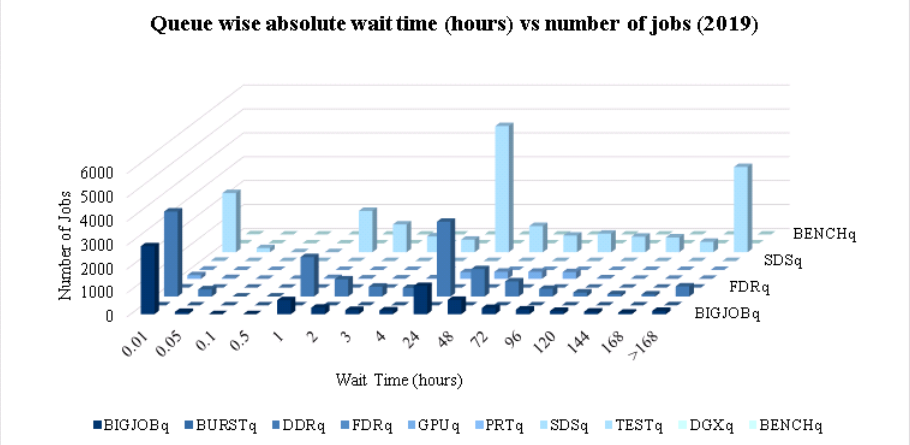
The jobs wait time / execution time ratio is more in incase of TESTq because of less walltime limit and limited resources available in TESTq.

Table: Queue wise Wait Time/Execution distribution

	Wait Time / Execution Time ratio	
Queue	**Wait time/execution time 2018**	**Wait time/execution time 2019**
BIGJOBq	3.621942632	7417.7135
BURSTq	1.535514368	2632
DDRq	2.342291109	403471388.7
FDRq	11.01225758	0.2201
DGXq	0	6.236
GPUq	1.012989407	1203296.869
PRTq	1.301004565	166133.798
SDSq	0.194288753	548.4633
TESTq	14.43705503	784485777.9
BENCHq	0	7417.7135

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





The above 3D plot shows distribution of number of jobs by wait time binned by queues. The wait time of the DDRq (jobs requiring less than 65 cores) is more due to availability of limited compute nodes under DDRq to promote capability computing.

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

Table: Queue wise absolute wait time (Hours) vs number of jobs (2019)

2019	0.01	0.05	0.1	0.5	1	2	3	4	24	48	72	96	120	144	168	>168
BIGJOBq	2845	96	0	0	588	275	179	158	1182	600	262	198	140	107	64	141
BURSTq	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	4
DDRq	3553	298	0	0	1646	719	411	359	3130	1147	631	320	167	102	85	422
FDRq	3	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
GPUq	154	29	0	0	32	15	12	17	279	296	293	278	21	1	0	0
PRTq	12	1	0	0	2	0	0	0	2	4	0	3	0	0	0	3
SDSq	13	2	0	0	2	2	1	0	0	0	0	0	0	0	0	0
TESTq	2477	175	0	0	1731	1163	663	527	5281	1096	698	779	651	620	436	3567

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5

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.

5.1 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-F & 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

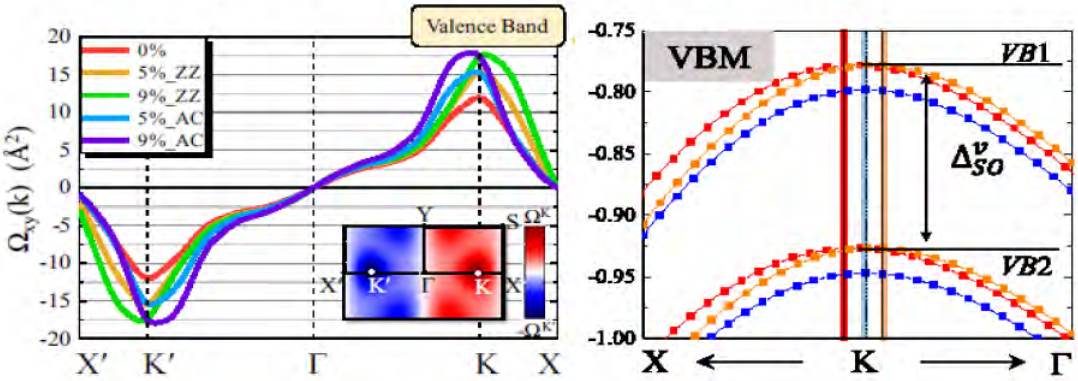
Research Challenge/s:

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)

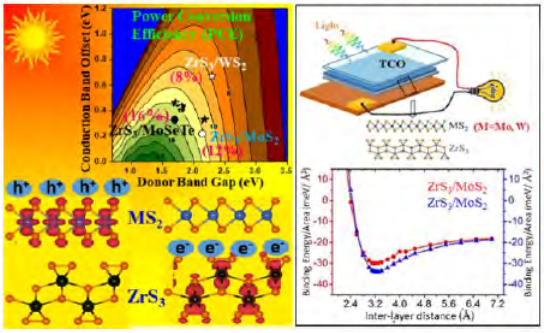
Work carried , Milestone, Achievements & Graphs, Plots: Presented Invited talk; Published papers; Students have presented posters in Conferences. Our papers published in the journal of Applied Surface Science, Physical Review B, Nanoscale, ACS applied materials interfaces, Journal of Materials Chemistry A etc.

Prof. Abir De Sarkar & Group

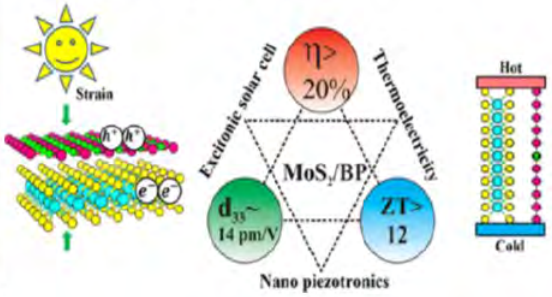
Valley drift and valley current modulation in strained monolayer MoS_2



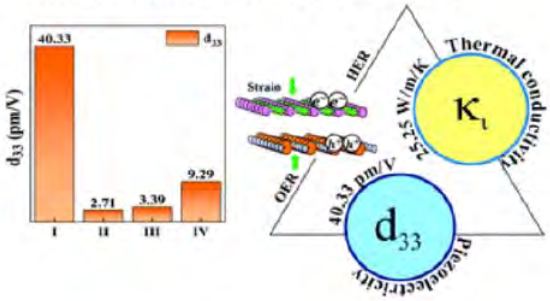
ZrS3/MS2 and ZrS3/MXY (MMo, W; X, YS, Se, Te; X ≠ Y) type-II van der Waals hetero-bilayers: Prospective candidates in 2D excitonic solar cells



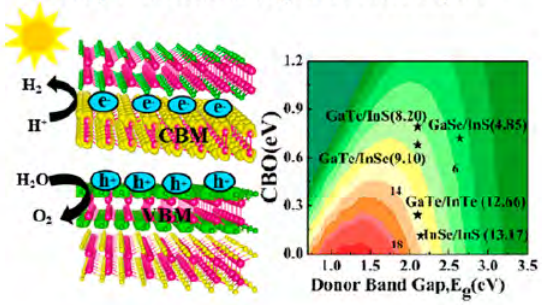
Interfacing Boron Monophosphide with Molybdenum Disulfide for an Ultrahigh Performance in Thermoelectrics, Two-Dimensional Excitonic Solar Cells, and Nanopiezotronics



Superhigh out-of-plane piezoelectricity, low thermal conductivity and photocatalytic abilities in ultrathin 2D van der Waals heterostructures of boron monophosphide and gallium nitride



Solar Energy Harvesting in Type II van der Waals Heterostructures of Semiconducting Group III Monochalcogenide Monolayers



Publications / Articles etc. (If any):

1. Manish Kumar Mohanta, Ashima Rawat, Nityasagar Jena, Dimple, Raihan Ahammed, Abir De Sarkar*, "Interfacing boron monophosphide with molybdenum disulphide for an ultrahigh performance in thermoelectrics, 2D excitonic solar cells and nanopiezotronics", ACS Applied Materials Interfaces, 12 (2020) 3114-3126 (Impact Factor 8.45)

2. Taniya Purkait, Raihan Ahammed, Abir De Sarkar, Ramendra Sundar Dey, "The role of exfoliating solvents for control synthesis of few-layer graphene-like nanosheets in energy storage applications: Theoretical and experimental investigation", Applied Surface Science 509 (2020) 145375 (Impact Factor 5.15)

3. Raihan Ahammed, Ashima Rawat, Nityasagar Jena, Dimple, Manish Kumar Mohanta, Abir De Sarkar*,"ZrS3/MS2 and ZrS3/MXY (M=Mo, W; X, Y=S, Se, Te; X Y) type-II van der

Waals hetero-bilayers: Prospective candidates in 2D excitonic solar cells", Applied Surface Science, 499 (2020)143894 (Impact Factor 5.15)

4. Manish Kumar Mohanta, Ashima Rawat, Dimple, Nityasagar Jena, Raihan Ahammed, Abir De Sarkar*, "Superhigh out-of-plane piezoelectricity, low thermal conductivity and photocatalytic abilities in ultrathin 2D van der Waals heterostructures of Boron Monophosphide and Gallium Nitride", Nanoscale 11 (2019) 21880-21890 (Impact Factor 6.97)

5. Nityasagar Jena, Dimple, Raihan Ahammed, Ashima Rawat, Manish Kumar Mohanta, Abir De Sarkar*,"Valley drift and valley current modulation in a strained monolayer MoS2", Physical Review B 100, 165413 (2019) (Impact Factor 3.74)

6. Ashima Rawat, Raihan Ahammed, Dimple Sharma, Nityasagar Jena, Manish Kumar Mohanta, Abir De Sarkar*, "Solar Energy Harvesting in Type II van der Waals Heterostructures of Semiconducting Group III Monochalcogenide Monolayers", Journal of Physical Chemistry C, 123 (2019) 12666-12675 (Impac Factor 4.31)

7. Manisha Das, Nityasagar Jena, Taniya Purkait, Navpreet Kamboj, Abir De Sarkar, Ramendra Sundar Dey, "Single-phase Ni5P4-Copper foam superhydrophilic and aerophobic core-shell nanostructures for efficient hydrogen evolution reaction", Journal of Materials Chemistry A, 7(2019)23989-23999 (Impact Factor 10.73)

Awards (If any):

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

- My PhD student (SRF), Miss Ashima Rawat has been awarded the Best Poster Award (two times) at two ACS sponsored Conferences, ICAN-2019 ICANN-2019 held at IIITM, Gwalior and IIT, Guwahati between 27-29 January, 2019 and 18-21 December, 2019 respectively
- Miss Ashima Rawat has participated in Computational School on Electronic Excitations in Novel th st Materials Using the Yambo Code held in ICTP, Trieste, Italy between 27 and 31 January, 2020 with travel support (640 Euro) and Health Insurance covered
- My student Nityasagar Jena has been offered a prestigious Postdoc position funded by the European Unions Graphene Flagship project, Horizon 2020, between Germany, France and Belgium. It happens to be the biggest scientific research initiative in Europe with a budget of ¿ 11 billion. He will submit his Ph.D. thesis shortly.

- My student Dimple has completed his PhD on 11.11.2019 and has joined as a prestigious CNRS Postdoctoral Fellow in Nancy, France on 20.11.2019
- I have been promoted to Professor/Scientist F at the Institute of Nano Science and Technology.

Appreciation / Recognition (if any):

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

I have presented an Invited talk at an ACS sponsored Conference titled International Conference on Advances in Nanomaterials and Devices for Energy and Environment (ICAN-2019) held in IIITM, Gwalior between 27-29 January, 2019.
Presented a talk at the 10th International Conference on Materials for Advanced Technologies (ICMAT- 2019) held in Singapore between 23 - 28 June, 2019

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: 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

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:

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

Publications / Articles:

1. Mohammad Ubaid, BS Pujari and A Aziz, "Adsorption of Na atom on mono-layer gallenene", AIP Conference Proceedings, 2142 (2019) 110021.
2. Mohammad Ubaid, BS Pujari and A Aziz, "First principle study of In/Ga-doped phosphorene",AIP Conference Proceedings, 2115 (2019) 030392.

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 (POSTER) a paper entitled Adsorption of Na atom on Mono-Layer Gallenene inInternational Conference on Advances in Basic Sciences (ICABS-19) February 7-9, 2019, G.D.C.Memorial College, Bahal (Bhiwani), Haryana, India.

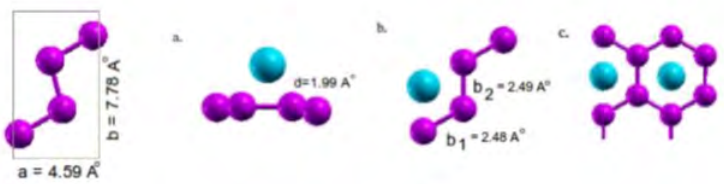


Figure 5.1: Top (a) and side (b) view of Na adsorbed mono-layer Ga 100 and the top (c) view of 2x2 Na adsorbed mono-layer Ga100.

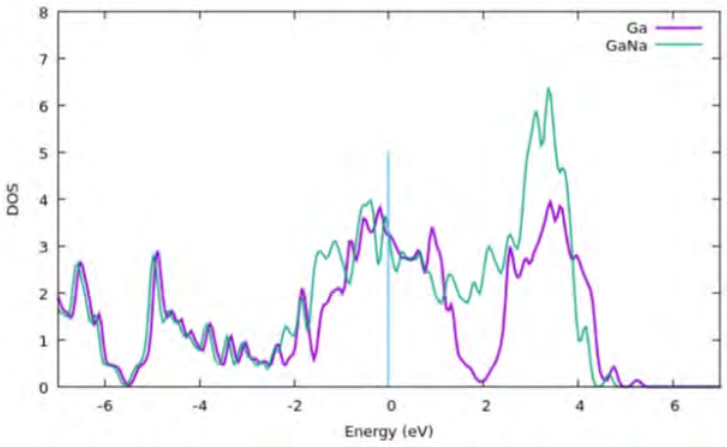


Figure 5.2: Electronic density of states of pristine and Na adsorbed Ga 100 (a) and of Na-Ga100.

2. Presented (POSTER) a paper entitled Electronic and Theraml Properties of In/Ga Doped Phosphorene: A DFT STUDY in an International Conference on Advanced Materials Centre for Nanoscience And Nanotechnology (ICAM-19) March 6-7, Jamia Millia Islamia (Central University), New Delhi.

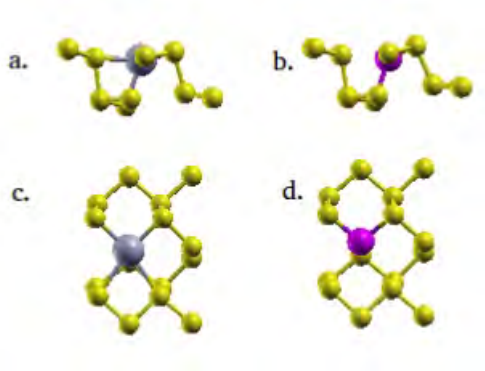


Figure 5.3: Side (a,b) and Top (c,d) views of In (a,c) and Ga (b,d)doped 2x2 phosphorene supercells.

Appreciation / Recognition (if any): No

References:

1. Geim, A. K. Novoselov, K. S. Nat. Mater. 2007 683191. 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 and 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):

Title of the work carried out: Two dimensional layered materials for toxic gas sensing applications using density functional theory based approaches.

Name & Designation of the Chief Investigator: Dr. Gaganpreet

E-mail Id: gaganpreet@iisermohali.ac.in

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

Research Challenge/s: Currently I am working on the below research areas Sensing of toxic gases using band gap engineered layered materials Water desalination using layered materials

Work carried , Milestone, Achievements & Graphs, Plots:

Sensing of toxic gases using band gap engineered layered materialsBand gap tuning is an efficient approach to modify the sensing ability of phosphorene. Herein, density functional theory (DFT) calculations have been performed to investigate the effect of various group elements (II-IVI) doping in phosphorene sheet for NH3 and NO2 gas sensing ability. The presence of NH3 and NO2 gas molecules on doped phosphorene nanosheet is found to alter the structural network, electronic properties hence leading to a better sensing and selectivity of the doped nanosheet. B doped phosphorene showed maximum adsorption of - 2.64 eV and -3.70 eV towards the NH3 and NO2 gas molecules respectively. NH3 adsorption on C, Si and S-doped phosphorene causes direct to indirect band gap transition while NO2 adsorption shows indirect band gap for pristine and S-doped phosphorene. Simulated scanning tunneling microscopy (STM) images showed different structural phases after gas adsorption due to electronic hybridization with orbitals from the upmost phosphorous atoms and the gas molecule. After gas adsorption, some flat bands are observedand localized states appear near the Fermi level, which are readily accessible at low bias voltages, thereby indicating the improved sensory functionality of doped phosphorene Water desalination using layered materials Desalination behavior through self-passivated phosphorene sheet is carried out

Publications / Articles etc. (If any):

1. Gaganpreet, Enhanced sensitivity of band gap engineered phosphorene towards NH3 and NO2 toxic gases, Applied surface Science, 50, 144967 (2019).

2. MunishShorie, Harmanjit Kaur, Gaganpreet Chadha, Kulvinder Singh, and Priyanka, SabherwalGraphitic Carbon nitride QDs impregnated biocompatible agarose cartridge for removal of heavy metals from contaminated water samples. J. of Hazardous Materials 367, 629 (2019).

Awards (If any):

1. Received International Travel grant from SERB, New Delhi for attending Graphene 2019 Conference at Rome, Italy

2. Received travel grant from CICS, Chennai for attending Graphene 2019 Conference at Rome, Italy

3. Best Ist Oral presentation award, at IEMPHYS-2019, held at IEM, Kolkata.

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

1. Oral Presentation, Toxic gas adsorption on doped phosphorene: A density functional approach, at IEMPHYS 2019 Kolkata November 2019.
2. Poster presentstaion, , Toxic gas adsorption on doped phosphorene: A density functional approach, Graphene 2019, Rome Italy

Appreciation / Recognition (if any):

References:

Benefits experience of using NPSF:

My research involves extensive simulations, maintenance of large data bases and data analysis for which I need very good computational facility. It is because of NPSF facility I am able complete my research projects within a given time. Moreover, the support provided by the NPSF team related to software installation, login issues etc. is really appreciable. I sincerely thanks CDAC Pune, for providing me allowing me the access and their impartial support.

Any other relevant information (if any):

Title of the work carried out: Strain Tunable Schottky Barriers and Tunneling Characteristics of Borophene/MX2 van der Waals Heterostructures

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

Student Researcher: Neha Katoch

E-mail Id: jgdish@cuhimachal.ac.in

Student Researcher email: nehakatoch2@gmail.com

Institution Name: Central University of Himachal Pradesh, Dharamshala, India

Research Challenge/s:

Novel Two Dimensional Structures beyond Graphene: A First Principle Study

Work carried , Milestone, Achievements & Graphs, Plots:

Based on first-principle calculations, we report the strain induced changes in electronic properties and their influence on current-voltage (I-V) characteristics of the borophene (12)/MX2 (M = Mo, W and X = S, Se) vdW heterostructures. The results reveal that the intrinsic electronic nature of borophene and MX2 is retained because of weak van der Waals interactions. However, p-type Schottky contacts are formed at the interface of the heterostructures. Application of the in-plane tensile and compression strains is effective in tuning the Schottky contacts and controlling the SBHs. Also, at the vertical pressure values of 5.46 and 5.25 GPa for 12/MoS2 and 12/WS2 respectively, Schottky contact changes from p-type to n-type. The I-V characteristics exhibit an ohmic behavior at low bias ±0.1V and noticeable NDR on changing positive (negative) biases. Such strain tunable Schottky barriers may be influential in 12/MX2 based high-performance nano- and optoelectronic devices.

Publications / Articles etc. (If any):

Neha Katoch, Ashok Kumar, Raman Sharma, P. K. Ahluwalia and Jagdish Kumar Strain Tunable Schottky Barriers and Tunneling Characteristics of Borophene/MX2 van der Waals Heterostructures Physica E: Low-dimensional System and Nanostructures, 113842 (accepted and in press). https://doi.org/10.1016/j.physe.2019.113842

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

Appreciation / Recognition (if any): No **References:** No

Benefits & experience of using NPSF:

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

Any other relevant information (if any): No

Title of the work carried out: Optical and thermoelectric properties of halide perovskites

Name & Designation of the Chief Investigator: Dr. K.C. Bhamu; PI-CUM-SERB-NPDF.

E-mail Id: kc.bhamu@ncl.res.in ; kcbhamu85@gmail.com

Institution Name: CSIR-NCL, Pune, NCL

Research Challenge/s: To tune the band gap and hence to improve optoelectronic and thermoelectric properties.

Work carried , Milestone, Achievements & Graphs, Plots:

We have predicted a significant band gap reduction from 3.3 eV to 0.65 eV by substitutional doping and its effect on opto-electronic and opto-thermoelectric properties from first principles study. The results predict that Sn/Pb and Ga Cu co-doping enhance the density of states significantly near the valence band maximum (VBM) and thus reduce the band gap by shifting the VBM upward while the alkali-metal (K/Rb) slightly increase the band gap. A strong absorption peak near ShockleyQueisser limit is observed in co-doped case while in Sn/Pb-doped case, we notice a peak in the middle of the visible region of solar the spectrum. The nature of band gap is indirect with Cu-Ga/Pb/Sn doping with a significant reduction in band gap, from 2.85 eV to 0.65 eV in the case of Ga-Cu co-doping. We observe a significant increase in the power factor (PF) (2.03mW/mK2) for n-type carrier concentration for Pb-doping, which is 3.5 times higher than the pristine case (0.6 mW/mK2) at 500 K.

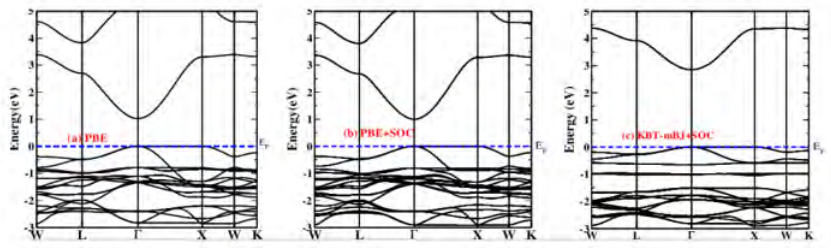


Fig. 1: Electronic dispersion relations of $Cs_2InAgCl_6$ using: (a) PBE (b) PBE+SOC, and (c) PBE with KTB-mBJ+SOC. The blue dash line represents the Fermi level (E_F).

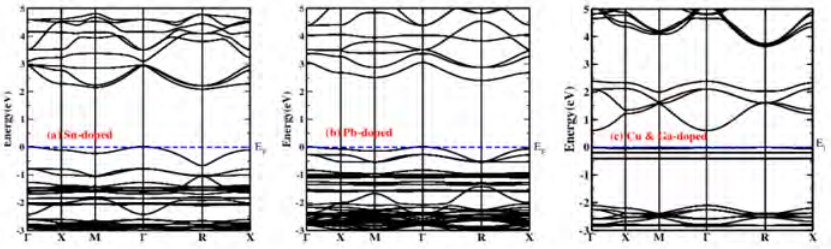


Fig. 2: Electronic dispersion relations of: (a) 25% Sn-doped, (b) 25% Pb-doped, and (c) 12.5% each Cu & Ga-doped $Cs_2InAgCl_6$ by using PBE functional with KTB-mBJ potential including SO effect. The blue dash line represents the Fermi level.

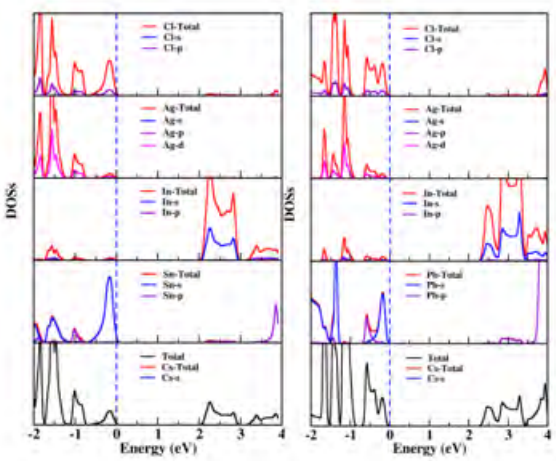


Fig. 3. Calculated total, atom, and orbital decomposed density of states of Sn- (Left panel) and Pb-doped (Right panel) Cs2InAgCl6 by using PBE functional with KTB-mBJ potential.

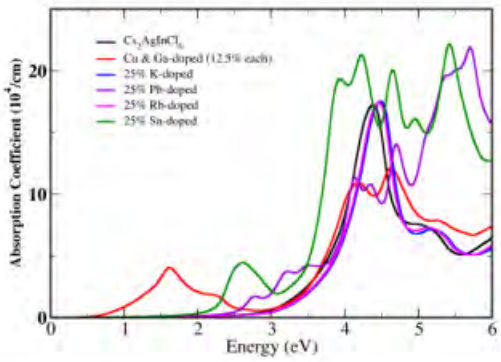


Fig. 4: Absorption coefficient of $Cs_2InAgCl_6$ along with doped cases as a function of photon energy.

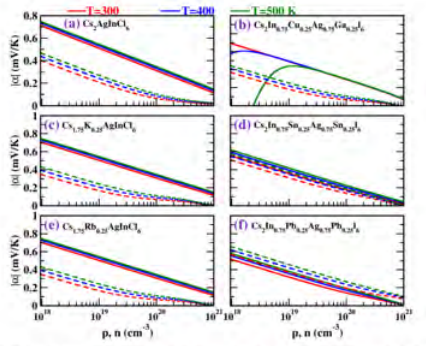


Fig. 5: The carrier concentration dependent Seebeck coefficient (|α|) at different temperatures for both *p*-type (solid) and *n*-type (dotted) of (a) $Cs_2AgInCl_6$, (b) Cu & Ga co-doped, (c) K-doped, (d) Pb-doped, (e) Rb-doped, and (f) Sn-doped.

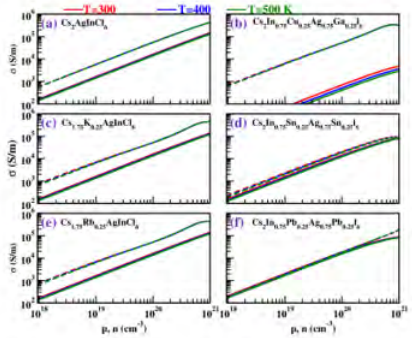


Fig. 6: Description is same as mentioned for Fig. 4 except the property which is electrical conductivity.

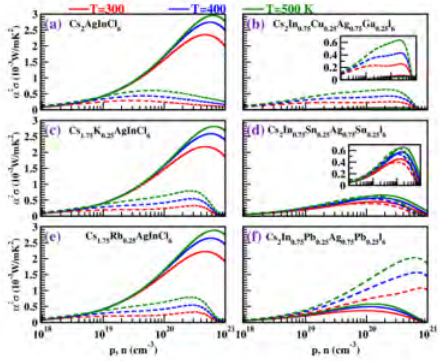


Fig. 7: Description is same as mentioned for Fig. 5 except the property which is power factor.

Publications / Articles etc. (If any):

1. Improving the Optical and Thermoelectric Properties of Cs2InAgCl6 with Substitutional Doping: A DFT Insight; arXiv:2001.07337 (2020).

2. Investigating effect of strain on electronic and optical properties of lead free double perovskite Cs2AgInCl6 solar cell compound: A first principle calculation; J. Alloys Compd. 817 (2020) 152758.

Awards (If any): Best Poster Presentation Award in ICRTENS-2019, Govt Science College Sikar (Raj.) during 12-13Feb, 2019.

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

Appreciation / Recognition (if any):-

References: As per in above mentioned published papers.

Benefits & experience of using NPSF:

Improving skill to deal some more complex systems

Any other relevant information (if any):-

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

Name & Designation of the Chief Investigator: Dr. Manikandan Paranjothy , Associate 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 at least 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, 2019 to December 31, 2019, we utilized the NPSF facility to carry out direct dynamics simulations on the following projects:(1) Theoretical investigation of the isomerization pathways of diazenes: torsion vs. inversion, (2) Competing Molecular and Radical Pathways in the Dissociation of Halons via Direct Chemical Dynamics Simulations. A brief summary of these works is given below:

Theoretical investigation of the isomerization pathways of diazenes: torsion vs. inversion: Diazenes are an important family of organic compounds used widely in synthetic and materials chemistry. These molecules have a planar geometry and exhibit cistrans isomerization. The simplest of all these molecules diazene (N2H2) has been subjected to several experimental and theoretical studies. Two mechanisms have been proposed for the cistrans isomerization of diazene, which are an in-plane inversion and an out-of-plane torsion. The activation energies for these pathways are similar and the competition between these two mechanisms has been discussed in the literature based on electronic structure theory calculations. Three decades ago, a classical dynamics investigation of diazene isomerization was carried out using a model Hamiltonian and it was indicated that the in-plane inversion is forbidden classically because of a centrifugal barrier and the out-of-plane torsion is the only isomerization pathway. In the present work, we investigated the cistrans isomerization dynamics of diazene using ab initio classical trajectory simulations at the CASSCF(2,2)/aug-cc-pVDZ level of electronic structure theory.

The simulation results confirmed the presence of the aforementioned centrifugal barrier for the inversion and torsion was the only observed pathway. The calculations were repeated for a similar system (difluorodiazene, N2F2) and again the centrifugal barrier prevented the inversion pathway.

Competing Molecular and Radical Pathways in the Dissociation of Halons via Direct Chemical Dynamics Simulations: A great deal of attention has been given to the decomposition chemistry of halons (halomethanes) due to their role in stratospheric ozone depletion. Knowledge of certain aspects of dissociation of halons such as the competition between radical and molecular pathways and their mechanistic details is limited. Halon molecules can isomerize to an iso form containing a halogenhalogen bond and such iso-halon forms have been identified as intermediates in condensed phase chemistry. Recently, a quantum chemistry study of role of iso-halons in the gas phase decomposition of halomethanes has been reported. In the present work, we have investigated the ground state dissociation chemistry of select halon molecules - CF2Cl2, CF2Br2, CHBr3, and CH2BrCl using electronic structure theory calculations and direct chemical dynamics simulations. Classical trajectories were generated on-the-fly using density functional PBE0/6-31G* level of theory at a fixed total energy. Simulation results showed that molecular products, in general, were dominant for all the four molecules at the chosen energy. A variety of mechanisms such as direct dissociation via multicenter transition states, decomposition via isomerization, radical recombinations, and roaming pathways contributed to the formation of molecular products. Atomic level mechanisms are presented, and the role of iso-halons in the gas phase chemistry of halomethanes is clearly established.

Publications / Articles etc. (If any):

1. Aarti Sindhu, Renuka Pradhan, Upakarasamy Lourderaj, Manikandan Paranjothy, " Theoretical investigation of the isomerization pathways of diazenes: torsion vs. inversion", Phys. Chem. Chem. Phys., 21, 15678-15685 (2019)

2. Sumitra Godara, Manikandan Paranjothy, " Competing Molecular and Radical Pathways in the Dissociation of Halons via Direct Chemical Dynamics Simulation", J. Phys. Chem. A, 123, 8527-8535(2019)

Awards (If any):

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

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:

1. Abstract

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]. A brief description of materials studied is as under:

1. $(Mn_xFe_{1-x})_2P_{1-y}Si_y$ [x,y = 0 or 1/3] alloys

Evaluating the prospects for new transition-metal rich rare-earth free permanent magnets, we have investigated the electronic and magnetic properties of Fe_2P and related Mn or/and Si-doped alloys using the full potential linearized augmented plane wave (FPLAPW) method under generalized gradient approximation (GGA) exchange correlation (XC) functional.

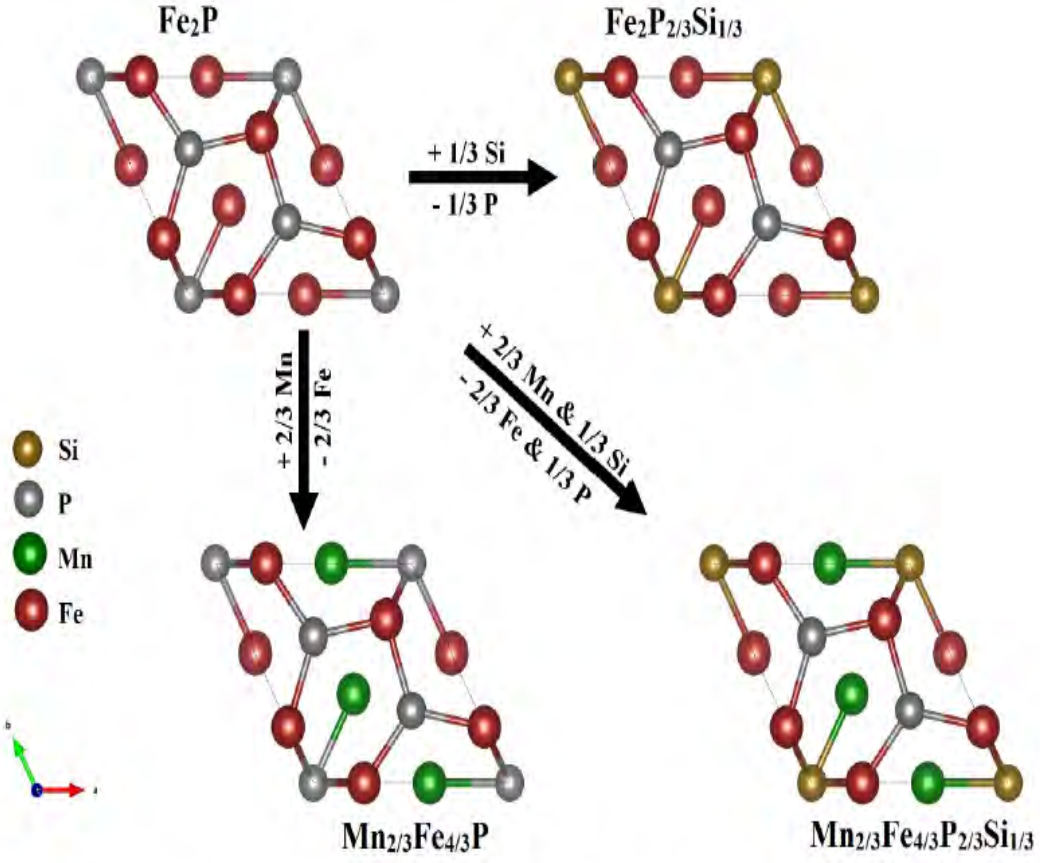


Fig. 1 Unit cell representation of hexagonal $(Mn_xFe_{1-x})_2P_{1-y}Si_y$ with (x,y=0 or 1/3) alloys

$(Mn_xFe_{1-x})_2P_{1-y}Si_y$ with x,y=0 or 1/3 yields four different alloys as shown in Fig.1. In pristine Fe_2P, the Fe_{3f}-P and Fe_{3g}-P bond lengths are found to be 2.294 Å and 1.983 Å, respectively, which are in agreement with the previous reports. A fruitful insight about the origin of magnetic moment and metallicity can be provided by computed total density of states (DOS). The spin polarized total DOS of studied alloys (Fig. 2) indicates that the metallic behavior is expected for all the cases. Further, for $(Mn_{1/3}Fe_{2/3})_2P$ and $(Mn_{1/3}Fe_{2/3})_2P_{2/3}Si_{1/3}$, a lower value of occupied minority DOS is clearly visible in the vicinity of Fermi level (E_F). Since the difference of occupied majority and minority DOS is proportional to the final spin moment appearing on the system, thus, Mn or/and P substitution leads to enhanced moment as compared to the parent compound, Fe_2P.

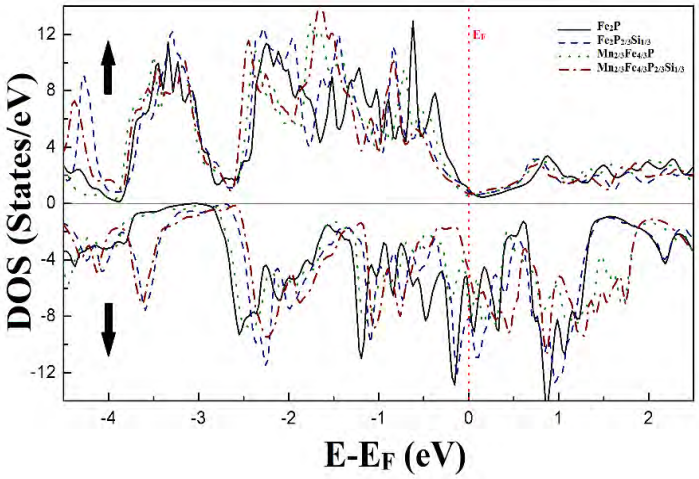


Fig. 2 Calculated spin-resolved total DOS per unit cell of hexagonal $(Mn_xFe_{1-x})_2P_{1-y}Si_y$ with (x,y=0 or 1/3) alloys

To calculate the MCA, the difference between equilibrium energy for magnetization along hard axis <100> and easy axis <001> is considered. Our calculated MCA for Fe_2P is 538 meV/f.u. (2.58 MJ/m^3). This is very close to experimental value, 538 meV/f.u. (2.32 MJ/m^3) [12] as compared to the previously calculated value (664 meV/f.u.) [13]. To obtain a better understanding of MCA, a careful analysis of electronic band structure near the E_F has been performed. To extract qualitative idea of the trends in MCA, we have restricted ourself to analyze the bandstructure only for majority spin. Fig. 3(a) and (b) show the band structures for Fe_2P and $(Mn_{1/3}Fe_{2/3})_2P_{2/3}Si_{1/3}$, respectively, along high symmetry directions in the Brillouin zone for majority spin only along <100> and <001> directions of magnetization. Since the SOC constant of 3d TMs is of the order of 0.05 eV and the states in the vicinity of E_F only can play an important role in deciding various properties of the materials, we have examined mainly the bandstructure near E_F, which clearly shows that change in splitting of energy bands when magnetization direction change from <001> to <100>.

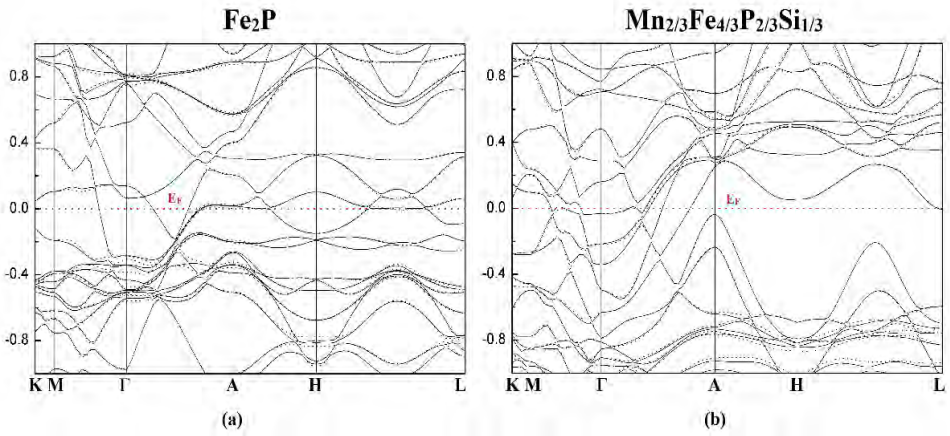


Fig. 3 Majority-spin Bandstructure of (a) Fe_2P and (b) $(Mn_{1/3}Fe_{2/3})_2P_{2/3}Si_{1/3}$ including spin-orbit coupling for magnetization axis along <100> (solid lines) and <001> (dotted lines) crystallographic axis. E_F is shifted to 0 eV for both cases.

Further, the k-point resolved MCA plotted along high symmetry points in Fig. 4 as a difference of the changes in band energies for magnetization direction <100> and <001>. For Fe_2P, the overall difference comes out to be positive. In $(Mn_{1/3}Fe_{2/3})_2P_{2/3}Si_{1/3}$, the substitution of Mn and Si atoms at their respective sites leads to different consequences that results in significant change in the band energies at all the symmetry points in Brillouin zone which is clearly visible in Fig. 3(b). Moreover, the changes in band energies for magnetization to arrive at <100> direction from that along <001> direction is almost inverted (from symmetry point G to A and H to L) that results in reduction of MCA as compared pristine Fe_2P. However, the overall difference comes out to be positive with lower magnitude.

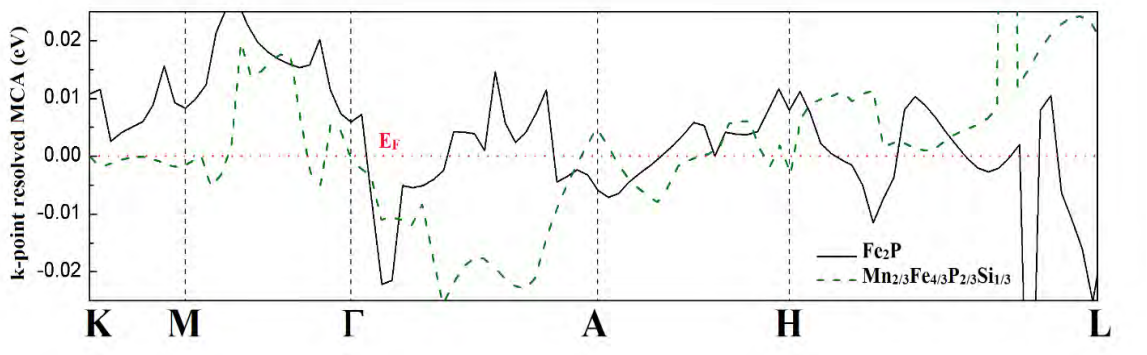


Fig. 4 Fe_2P and $(Mn_{1/3}Fe_{2/3})_2P_{2/3}Si_{1/3}$, k-point resolved MCA along high symmetry directions. E_F is shifted to 0 eV

Table 1. Calculated MCA (in units of meV/f.u. and MJ/m^3), nature of MCA, maximum energy product ($(BH)_{max}$), magnetization (M_s), coercive field (H_c) and magnetic hardness parameter (κ) of all the considered systems

Systems	MCA (μeV/f.u.)	(MJ/m^3)	Nature	$(BH)_{max}$ (kJ/m^3)	M_s (MA/m)	H_c (MA/m)	κ
Fe_2P	538	2.58	Uniaxial	219.52	0.84	4.91	1.81
	500[12]	2.32[12]	Uniaxial	-	-	-	-
	664[13]	-	Uniaxial	-	-	-	-
$Fe_2P_{2/3}Si_{1/3}$	454	2.12	Uniaxial	267.93	0.92	3.95	1.46
$(Mn_{1/3}Fe_{2/3})_2P$	389	1.83	Uniaxial	327.81	1.02	2.84	1.23
$(Mn_{1/3}Fe_{2/3})_2P_{2/3}Si_{1/3}$	316	1.45	Uniaxial	381.81	1.10	2.09	1.01

We note that the $(BH)_{max}$ and M_s are enhanced significantly on Mn or/and Si substitution. The predicted $(BH)_{max}$ values of all the doped compounds are good enough for these to qualify as PMs, since larger the energy product $(BH)_{max}$, more is the energy stored in the PMs. In $(Mn_{1/3}Fe_{2/3})_2P_{2/3}Si_{1/3}$, although MCA reduces but its hardness parameter, $\kappa > 1$, therefore, its hard magnetic behaviour remains preserved and $(BH)_{max}$ is almost 50% higher as compared to that for parent compound Fe_2P. In totality, a large value of magnetic moment and considerable MCA along with a large $(BH)_{max}$ make the resultant alloy an even better candidate for RE free permanent magnets and spintronics applications than Fe_2P.

2. Hybrid halide perovskite Cs:FAPbI$_3$

Hybrid halide perovskites (HHPs) have revolutionized the scenario of emerging photovoltaic technologies with recently certified photon conversion efficiency (PCE) of 22% [14]. This steep rise in the PCE from 3.8% [15] in 2009 to present value has never been seen before in any other existing solar cell technology. Due to the enormous value of research interests in this field, current performance of HHP solar cells is further expected to increase substantially. The reasons for the progress in HHP solar cells are their easy fabrication from the liquid phases [16] and the efficiency which can be tuned by controlling their structural order and composition [17]. HHPs have standard AMX_3 perovskite structure, where X is the halide anion (Cl^-, Br^-, I^-), M is the metal cation (Ge, Sn, Pb), while the position A is taken by an organic molecule, commonly methylammonium, CH_3NH_3 (MA) and formamidinium, $HC(NH_2)_2$ (FA) etc. $MAPbI_3$ has been extensively used in HHP solar cells because of excellent properties like direct bandgap of 1.55 eV [18], small exciton binding energy [19], high level of defect self regulation [20], long charge carrier diffusion length [21] and excellent carrier mobility [22]. But lack of intrinsic long term stability in $MAPbI_3$ makes it a poor choice for stable solar cells [23]. So there is a pressing need to look for new HHP materials that are both stable as well as efficient in operating conditions. $FAPbI_3$ can be an alternative to $MAPbI_3$ due to its superior photostability [24]. An intuitive strategy to further enhance the stability in the HHP absorber layer can be to dope some percentage of cation A by suitable dopant such that the stability is achieved and excellent photovoltaic properties are also not compromised. Keeping Goldschmidt tolerance factor in consideration FA^+ can be easily substituted by Cs^+ without destroying the Pb-I octahedral arrangement. For this, first principles calculations were carried out using PAW as implemented in VASP code [10] to systematically examine the geometry, electronic structure and optical properties of 12.5% of Cs-doped $FAPbI_3$ (Cs:$FAPbI_3$) perovskite.

$FAPbI_3$ adopts a cubic structure with space group Pm-3m at room temperature [25]. In a unit cell of $FAPbI_3$ each Pb atom coordinates with six I-atoms (four in equatorial and two in apical direction. From the experimental observations, the FA^+ cation reorients quite rapidly [0.5-14 ps] inside the PbI_6-octahedron cage at the room temperature [24]. However for computation, the FA^+ cation has been relaxed to a fixed orientation. We used experimental lattice parameters [23] as the input parameters of our DFT calculations to obtained the optimized local structure of $FAPbI_3$.

In order to obtain 12.5% of Cs doping, a 2×2×2 supercell was formed and one FA^+ ion was replaced by Cs^+ within the supercell (Fig. 5). Doping concentration beyond 12.5% has been avoided as increased Cs content would have undesirably enhanced the bandgap value.

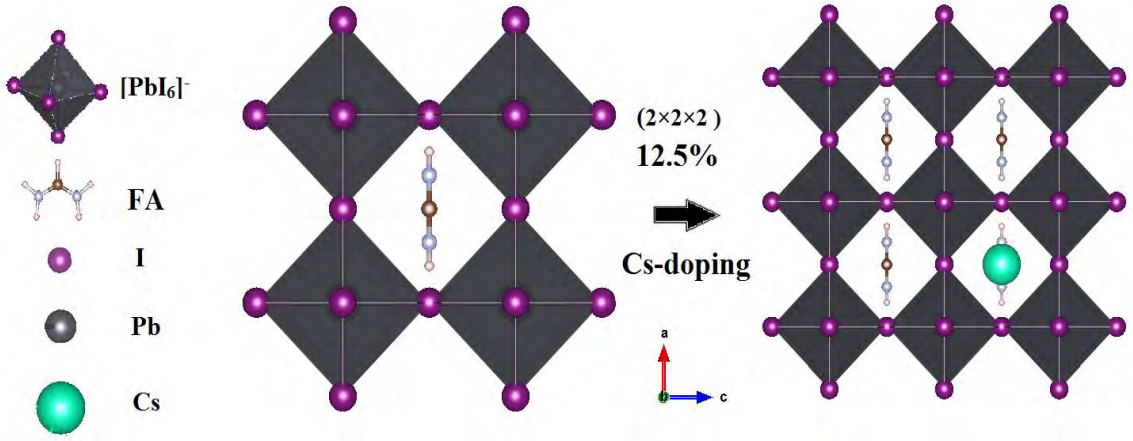


Fig. 5. Schematics for introducing 12.5% of Cs-doping in $FAPbI_3$.

The optimized lattice parameters of pure and Cs:$FAPbI_3$ obtained after relaxation are listed in the Table 2 which are in good agreement with experimental values [25] and other theoretical data [27]. The incorporation of smaller Cs in $FAPbI_3$ 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:$FAPbI_3$ HHP.

Table 2. Calculated lattice parameters of $MAPbI_3$ and Cs:$MAPbI_3$

	$FAPbI_3$	Cs:$FAPbI_3$
	a (in Å)	a (in Å)
This work	6.54	6.50
Experiment [25]	6.36	-
Theory [27]	6.36	-

The magnitude of band gap of absorber material is related to the maximum voltage of the PV device and determines the optical absorption. The electronic band structures of $FAPbI_3$ and Cs:$FAPbI_3$ along high symmetry points of the Brillioun zone reported in Fig. 6. The fundamental bandgap (E_g) of 1.47 eV is obtained between valence band maxima (VBM) and conduction band minima (CBM) along the R- R direction in $FAPbI_3$ which is in good agreement with experimental value of 1.48 eV [25]. 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 E_g 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.

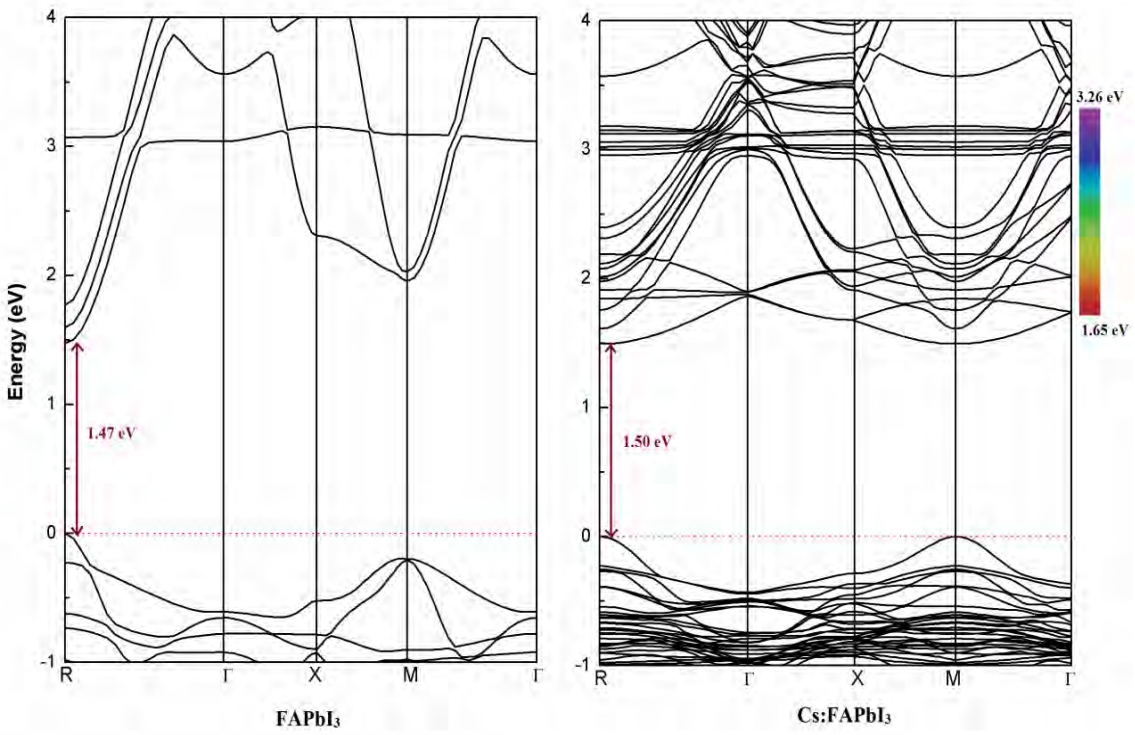


Fig. 6. Bandstructure of $FAPbI_3$ and $Cs:FAPbI_3$ along some high symmetry points of the Brillioun zone.

To understand the bonding mechanism between the atoms of the $Cs:MAPbI_3$, the analysis of partial density of states (PDOS) was performed (Fig. 7). VBM is constituted of combination of Pb-6s and I-5p states whereas the CBM is formed by the empty Pb-6p states along with a residual contribution from I-5p states. FA^+ cation do not contribute directly to the band edges. Likewise the major contribution of Cs is around -7.5 eV i.e. deep inside the valence band.

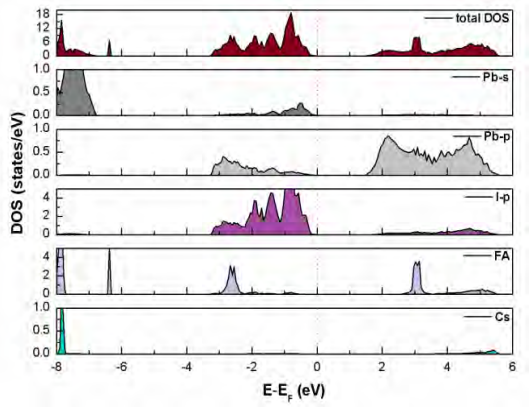


Fig. 7. Calculated Partial DOS (PDOS) of $Cs:FAPbI_3$ at GGA level of theory.

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 as governed by Fig. 7. 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. Moreover, the value of absorption coefficient in $Cs:FAPbI_3$ is higher than that of $FAPbI_3$ in the visible energy range i.e. from 1.62 eV to 3.25 eV making it one of the potential candidates for the absorber layer in PSCs.

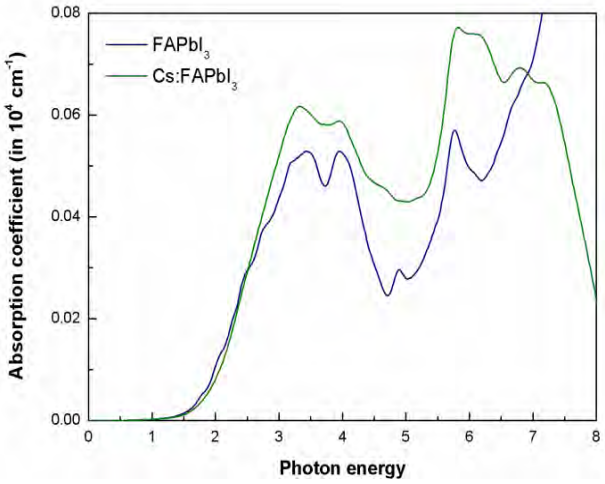


Fig. 8. Absorption coefficient of $FAPbI_3$ and $Cs:FAPbI_3$.

Thus our results show that decreased cubo-octahedral volume post Cs-doping not only impart the stability to FAPbI3 but also increased the value of bandgap to 1.50 eV.

3. Pb-Free Halide Double Perovskite $Cs_2BiAgBr_6$

Identifying a stable and non-toxic perovskite optoelectronic material with band gap, carrier mobility in the approximation of extensively used $CH_3NH_3PbI_3$ ($MAPbI_3$) perovskites, is one of the key challenges to be addressed in the area of perovskite solar cells. The replacement of Pb^{2+} with Sn^{2+} seems an obvious option but due to instability of Sn-based perovskite, it is highly unlikely that Sn-based perovskite solar cells will ever have commercial viability [28]. Different configurations of ionic charges in $A^+M^{2+}X_3$ formula does not provide much hopes as alternatives for lead based perovskites in solar cells. On the other hand, if search is expanded from ternary $A^+M^{2+}X_3$ perovskites to quaternary $A_2M^+M^{3+}X_6$ double perovskites, there can be many possible combination of M^+ and M^{3+} to obtain suitable electronic and optical properties. These types of compounds are abundant and are well known for their ferroelectric, ferromagnetic and multiferroic properties. In double perovskites, M^{3+} are chosen from pnictogens and Bi and Sb can be most suitable choices whereas for monovalent cations noble metals like Cu, Ag and Au can be considered. In this regard, we documented the structural, electronic and optical properties of Pb-free perovskite $Cs_2BiAgBr_6$ using FPLAPW method as implemented in WIEN2k[11] package.

$Cs_2BiAgBr_6$ is a three-dimensional framework of corner connected octahedra and Cs^+ ions occupying the cuboctahedral cavities in the framework (Fig. 9). The double perovskite structure is then obtained by alternating Ag^+ and Bi^{3+} centered octahedra, with each Ag/ Bi atom coordinating with six Br-atoms (four in equatorial and two in apical direction), in all three directions, building up a superstructure that is typically referred to as rock salt ordering (Fig. 10). Bond distances are tabulated in Table 3. Due to smaller electronegativity of Ag^+ than Bi^{3+} the Ag-Br distances are slightly shorter than the Bi-Br distances. Moreover, no octahedral titling is observed in $Cs_2BiAgBr_6$.

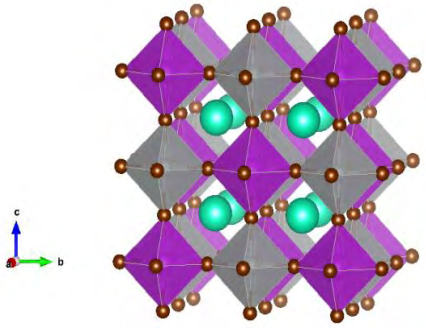


Fig. 9. Conventional unit cell of $Cs_2BiAgBr_6$. Here grey/purple/brown/turquoise sphere represents Ag/Bi/Br/Cs atom. Ag and Bi centered octahedra are shown as grey and purple polyhedral, respectively.

Table 3. Bond lengths among various atoms in$Cs_2BiAgBr_6$

Bond lengths (Å)	
Cs-Br	4.065
Ag-Br	2.750
Bi-Br	2.841

The analysis of total DOS reveals that the XC functionals have insignificant effects on the main characteristics of peaks nevertheless their impact is significantly observed on energy bandgap values (Fig. 10) since the conduction band is shifted towards higher energies within mBJLDA as compared to GGA. For $Cs_2BiAgBr_6$ GGA gave an underestimated value of 1.17 eV for the fundamental band gap whereas a more reliable value of 2.01 eV was obtained using mBJLDA, which is in good agreement with the experimental value of 2.19 eV [29].

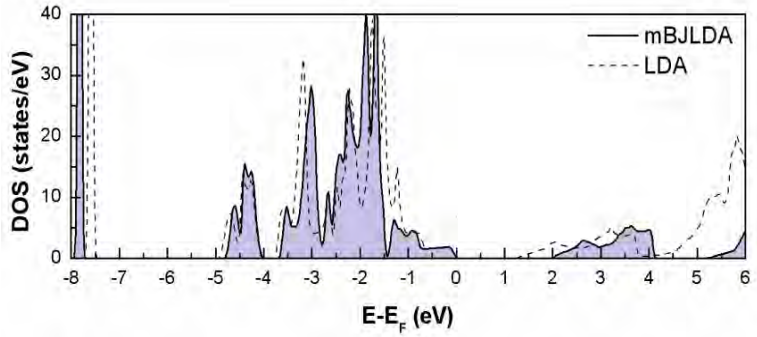


Fig. 10. Calculated total Density of states (DOS) of $Cs_2BiAgBr_6$ within GGA and mBJLDA

To understand the bonding mechanism between the atoms of $Cs_2BiAgBr_6$, the analysis of partial density of states (PDOS) was performed (Fig. 11a). The valence band (VB) is majorly contributed from Br-4p along with extensive ad mixture of Ag-4d states. There exists hybridization between Ag-4d and Br-4p states at valence band maxima (VBM). On the other hand, conduction band (CB) is formed from contribution from Ag-5s and Bi-4p states mainly. The valence to conduction band transitions is primary from Br-4p states to Ag-5s and Bi-4p states.

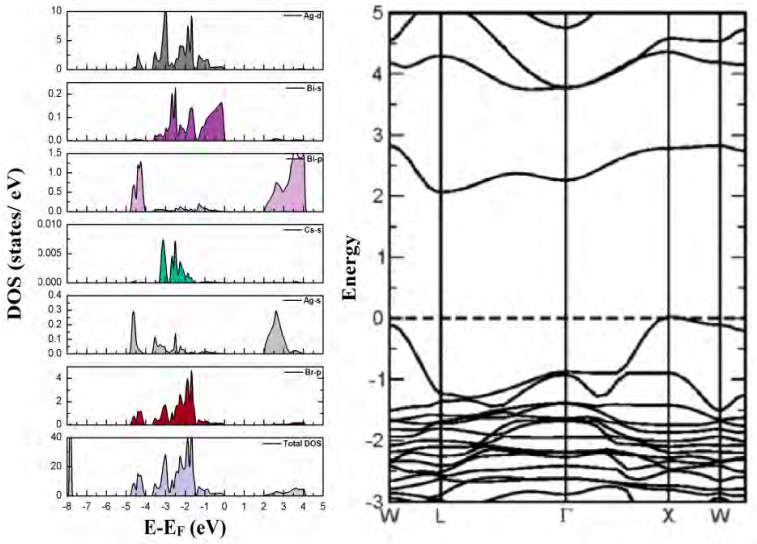


Fig.11. Partial DOS and band structure of $Cs_2BiAgBr_6$ along high symmetry points in Brillioun zone

The electronic band structure of $Cs_2BiAgBr_6$ at high symmetry points in the Brillioun zone were analyzed in Fig. 11(b). It has indirect band gap with VBM at X point whereas the CBM is located at L point. The participation of both Ag and Bi states in the lower energy conduction band is the reason for dispersion in these bands. The presence of Ag-4d states, which are highly directional in the VB, is partially responsible for the indirect nature of band gap in this material. The lowest direct transition occurs at X. Moreover, relatively flat bands are observed in the energies between

-1.5 eV to -3 eV. The linear absorption spectrum of $Cs_2BiAgBr_6$ is depicted in Fig. 12. The absorption onset is striking similarity between this spectrum and that of corresponding HHP $MAPbBr_3$[30], apart from some minor differences seen in the photon energy above the absorption onset. However, in present case, the onset of absorption is not quite sharp which can be attributed to the indirect nature of band gap in $Cs_2BiAgBr_6$.

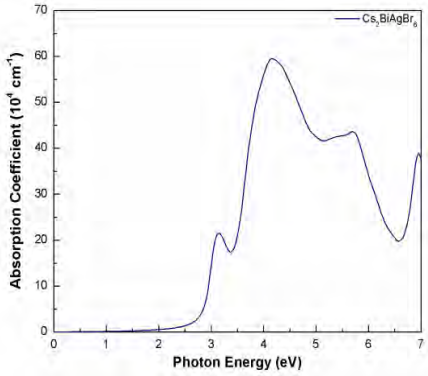


Fig. 12. Calculated linear absorption spectra of $Cs_2BiAgBr_6$

Thus, the linear absorption spectrum of double perovskite $Cs_2BiAgBr_6$ shows the striking similarity to that of mainstream HHP like $MAPbBr_3$, making it one of the promising absorber layer material in non-toxic and stable perovskite-based solar cells.

4. $M_2Ni_{21}B_6$ and $M_3Ni_{20}B_6$ (M = U, Nb) compounds

According to previous reports, U with Ni and B, forms $U_2Ni_{21}B_6$ ($W_2Cr_{21}C_6$-type) [31], while Nb forms both the $Nb_2Ni_{21}B_6$ ($W_2Cr_{21}C_6$-type) [32] and $Nb_3Ni_{20}B_6$ ($Mg_3Ni_{20}B_6$- type) [33] phases. Therefore, we have investigated samples with nominal composition "$U_2Ni_{21}B_6$", "$U_3Ni_{20}B_6$", "$Nb_2Ni_{21}B_6$", and "$Nb_3Ni_{20}B_6$" to study the formation, crystal chemistry, and physical properties of these phases via DFT calculations in order to provide a deeper understanding of the structure property relationships in these compounds.

DFT calculations for the synthesized $M_2Ni_{21}B_6$ and $M_3Ni_{20}B_6$ (M = U, Nb) compounds were performed by using the full-potential linearized augmented plane-wave (FPLAPW) method as implemented in the WIEN2k package [11]. For Nb-based systems, a generalized gradient approximation (GGA) under Perdew−Burke−Ernzerhof (PBE) parametrization [34] was used as the exchange-correlation functional. On the other hand, for U-based systems, Coulomb correction in GGA with inclusion of the Hubbard U parameter for onsite U-5*f* electron correlation was also made. The effective potential used for this purpose was $U_{eff} = U - J$, where onsite Coulomb Interaction U = 4.50 eV and exchange parameter J = 0.51 eV, as suggested in recent work on a U compound [35]. The spin−orbit coupling was included as a second variational step approach in both GGA and GGA+U formalisms [36]. The fixed-spin-moment (FSM) calculations were used to obtain the magnetic moment (≈10 μ_B) on the intermediate compound $Nb_{2.5}Ni_{20.5}B_6$. With the FSM approach, it is possible to constrain the total spin magnetic moment per unit cell to a fixed value and thus force a particular ferromagnetic solution. This is particularly useful for systems with several metastable magnetic solutions, where conventional spin-polarized calculation would not converge or the solution may depend on the starting density.

The experimental results showed that the stable crystallographically ordered compounds are $U_2Ni_{21}B_6$ and $Nb_3Ni_{20}B_6$, while $U_3Ni_{20}B_6$ and $Nb_2Ni_{20}B_6$ do not form. To provide a better understanding of these experimental observations, DFT-based total energy calculations using the FPLAPW method were performed and the formation energies for all four studied compounds were evaluated. $U_3Ni_{20}B_6$ and $Nb_2Ni_{20}B_6$ were found to have formation energies of 2.87 and 3.17 meV/cell, respectively. Such positive values of the formation energies indicate the instability of both compounds; this result is in agreement with the experimental observation. For the other two compounds, i.e., $U_2Ni_{21}B_6$ and $Nb_3Ni_{20}B_6$, the obtained formation energies are −2.85 and −1.52 meV/cell, respectively, which support the structural stability of these phases and corroborate our experimental study.

The total DOS of the stable compounds ($U_2Ni_{21}B_6$ and $Nb_3Ni_{20}B_6$) has been analyzed and is depicted in Fig. 13. The DOS of these phases (Fig. 13(a) and 13(b)) are non-spin polarized, with almost identical contributions from spin-up and spin-down electrons. The DOS plots in Fig. 13 have been marked with separate colors to show the input

from the different atomic sites. The unoccupied DOS in the vicinity of EF for $U_2Ni_{21}B_6$ and $Nb_3Ni_{20}B_6$ is mainly contributed by the U-5f and Nb-4d states, respectively.

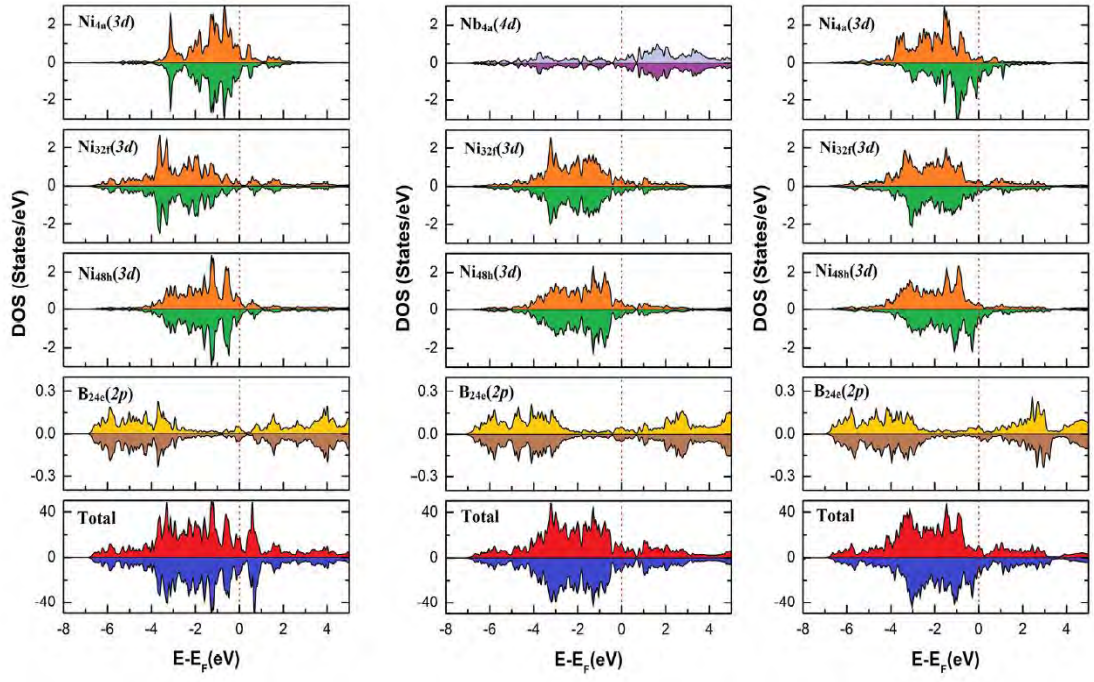


Fig. 13. Atoms resolved (4*a*, 8*c*, 32*f*, 48*h*, and 24*e* sites) and total DOS for (a) $U_2Ni_{21}B_6$, (b) $Nb_3Ni_{20}B_6$, and (c) hypothetical $Nb_2Ni_{21}B_6$ (the FSM case) compounds.

On the other hand, the DOS near E_F in the occupied region is an admixture of the 3d states of all Ni atoms. The B-2p states, although having a minimal contribution in the total DOS, play an important role in deciding the overall shape of the bands via p−d hybridization. Because for both compounds all of the individual atoms have nonpolarized DOS, the net magnetic moment appearing on the crystal as a whole is turning out to be almost zero. This observation validates the Pauli paramagnetic behavior found in $U_2Ni_{21}B_6$ and $Nb_3Ni_{20}B_6$. The experimental data obtained in the investigation of the intermediate compound $Nb_{2.5}Ni_{20.5}B_6$ prove that both Nb and Ni atoms occupy the 4a site in equal proportions (50%−50%). As in DFT simulations, it is not possible to consider partial occupancy of one site by two atoms; therefore, a different way of studying the magnetism observed in this compound had to be adopted. Via both the experimental and theoretical approaches, we have already shown that Nb in the 4a site in $Nb_3Ni_{20}B_6$ does not induce any magnetic exchange interaction.

In the hypothetical $Nb_2Ni_{21}B$ compound, a full occupancy of the 4a site by Ni atoms occurs. However, the actual compound that has to be simulated is $Nb_{2.5}Ni_{20.5}B_6$ (limit of the solid solution $Nb_{2+y}Ni_{20-y}B_6$) with a magnetic moment of 10 μ_B. Hence, to mimic this compound, the $Nb_2Ni_{21}B_6$ compound was considered, and FSM calculation generating a total moment of 10 μ_B was performed. By doing so, the states responsible for giving rise to this large moment in $Nb_{2.5}Ni_{20.5}B_6$ can be predicted. The DOS for $Nb_2Ni_{21}B_6$ (the FSM case) is shown in Fig. 13(c), which indicates the total DOS is spin-polarized in nature, with unequal contributions from the majority and minority spin channels.

To elucidate the chemical bonding and charge mechanism in the stable $U_2Ni_{21}B_6$ and $Nb_3Ni_{20}B_6$ compounds, the total valence electronic charge densities, n(r), along the (110) plane are analyzed using the XCrySDen program in Fig. 14. The behaviors of the charge densities of both compounds are almost identical, and no sudden change in these densities was observed with respect to each other. Along the (110) plane, two arrays of Ni atoms in $U_2Ni_{21}B_6$ or $Nb_3Ni_{20}B_6$ are sandwiched between two U−B or Nb−B layers and the sharing of electronic charge is visible along the

Ni−B bond, making this bond polar covalent. The charge-density distribution is essentially spherical around the Ni and U atoms. The contour plot of the electron density in $U_2Ni_{21}B_6$ indicates the maximum accumulation of charge around the U atom.

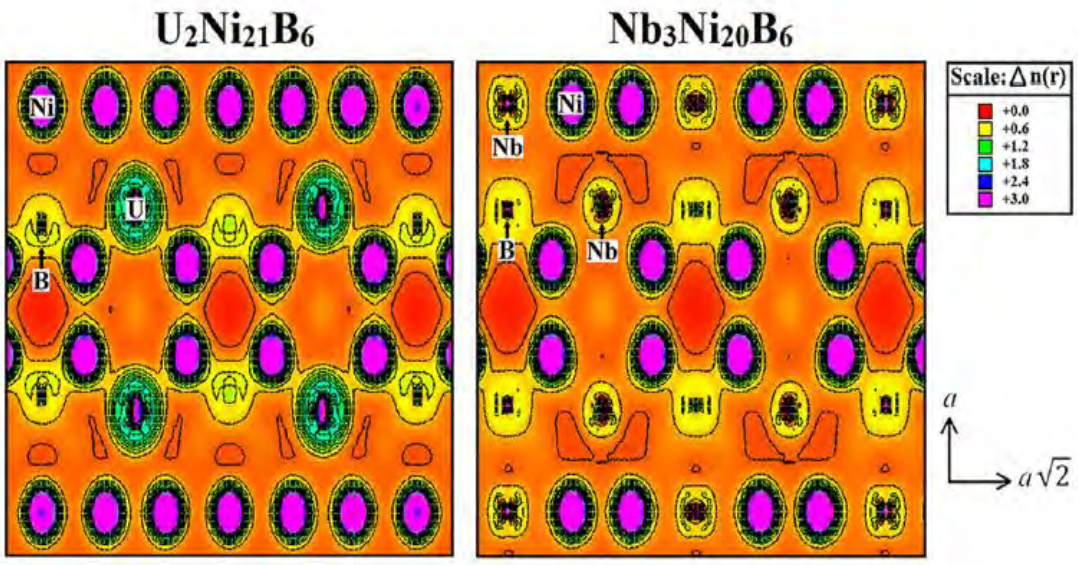


Fig. 14. Total valence electron charge density, n(r), in the (110) plane (in units of e/Å^3) for the stable $U_2Ni_{21}B_6$ and $Nb_3Ni_{20}B_6$ compounds.

Publications / Articles etc. (If any):

1. Stability, Crystal Chemistry, and Magnetism of $U_{2+x}Ni_{21-x}B_6$ and $Nb_{3-y}Ni_{20+y}B_6$ and the Role of Uranium in the Formation of the Quaternary $U_{2-z}Nb_zNi_{21}B_6$ and $U_\delta Nb_{3-\delta}Ni_{20}B_6$ Systems, Alessia Provino, Volodymyr Smetana, Timothy A. Hackett, Durga Paudyal, Manish K. Kashyap, Cristina Bernini, Amitava Bhattacharyya, Sudesh K. Dhar, Marcella Pani, Flavio Gatti, Anja-Verena Mudring, and Pietro Manfrinetti, Inorg. Chem. 58, 15045−15059 (2019).
2. First principles study of structural, electronic and optical properties of Cs-doped $HC(NH_2)_2PbI_3$ for photovoltaic applications, Ankur Taya, Renu Singla, Priti Rani, Jyoti Thakur, and Manish K. Kashyap, AIP Conference Proceedings 2115, 030610 (2019).
3. Structural, Electronic and Optical studies of Pb-Free Halide Double Perovskite $Cs_2BiAgBr_6$; an mBJLDA approach, Ankur Taya, Priti Rani and Manish K. Kashyap, AIP Conference Proceedings 2093, 020028 (2019).

Awards (If any):

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

1. Attended and presented a paper entitled “Electronic, structural, vibrational and magnetic properties of interstitially doped $L1_0$-FeNi:N Alloy” in 26th WIEN2k Workshop on DFT based simulations of solids with the WIEN2k code at TU, Wien, Vienna, Austria during 13-17 August, 2019.
2. Attended and presented a paper entitled “Effect of Cs doping on optical absorption of $APbI_3$ (A =-CH_3NH_3, -$CH(NH_2)_2$) hybrid lead iodide perovskites” in third International conference on advanced

materials (ICAM 2019) at Mahatma Gandhi University, Kottayam, Kerala during 09-11 August, 2019.

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 cannot be possible. We are fortunate to have C-DAC's 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 completed 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 the 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: Extraction of Caffeine and Its Effect on Neural Proteins: A Computer Simulation Study

Name & Designation of the Chief Investigator: Dr. Moumita Saharay, UGC-Assistant Professor, Department of Physics, Osmania University, Hyderabad 500007

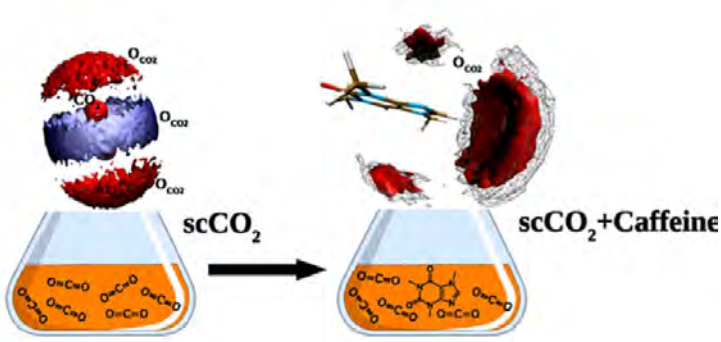
E-mail Id: saharaymou@gmail.com

Institution Name: Osmania University

Research Challenge/s:

The extraction of caffeine from green tea leaves and cocoa beans is a common industrial process for the production of decaffeinated beverages and pharmaceuticals [112]. The choice of the solvent critically determines the yield of this extraction process. Being an environmentally benign and recyclable solvent, supercritical carbon dioxide (scCO2) has emerged as the most desirable green solvent for caffeine extraction. The present study investigates the solvation properties of caffeine in scCO2 at two different temperatures (318 and 350 K) using molecular dynamics simulations. Unlike in water, the caffeine molecules in scCO2 do not aggregate to form clusters due to relatively stronger caffeineCO2 interactions. A wellstructured scCO2 solvent shell envelops each caffeine molecule as a result of strong electrondonoracceptor (EDA) and hydrogen bonding interactions between these two species. Upon heating, although marginal site-specific changes in the distribution of nearest CO2 around caffeine are observed, the overall distribution is retained. At a higher temperature, the caffeineCO2 hydrogen- bonding interactions are weakened, while their EDA interactions become relatively stronger. The results underscore the importance of the interplay of these interactions in determining stable solvent structures and solubility of caffeine in scCO2.

Work carried , Milestone, Achievements & Graphs, Plots:



We have studied the structure, energetics, and solvation properties of the caffeine-scCO2 mixture using molecular dynamics simulations. The model systems considered were based on the experimental data pertaining to the maximum solubility of caffeine at a particular density and temperature of scCO2. Unlike in the hydrated environment where caffeine molecules -stack with each other, the nonpolar scCO2 did not favor aggregation of caffeine molecules; most caffeine molecules existed in the monomeric form in scCO2 with a small fraction of hydrogen-bonded dimers. The gas phase calculations also showed that a pair of -stacked caffeine molecules was relatively less stable than a caffeineCO2 pair in isolation. Well-structured carbon dioxide solvation shells were formed around each caffeine molecule as a result of strong electrondonoracceptor

and hydrogen-bonding interactions between them. Although the present work was focused on the solvent structure around caffeine in pristine scCO2, it may serve as a baseline to understand the solvation properties of other purine alkaloids in scCO2 or other C=O-containing solvents and to investigate the effects of cosolvents such as ethanol and water on the solubility of caffeine in scCO2.

Publications / Articles etc. (If any):

Solubility of Caffeine in Supercritical CO2 : A Molecular Dynamics Simulation Study

Vishwanath Reddy, Moumita Saharay

The Journal of Physical Chemistry B, 2019, 123, 96859691, Impact factor 3

Awards (If any): NONE

Work presented in conference/s with photographs (if any):NONE

Appreciation / Recognition (if any): NONE

References:

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Benefits & experience of using NPSF:

We thank the NPSF facility for fast and efficient computing. The waiting time in the queue is nominal which is an added benefit of using this facility. We greatly appreciate the administration of NPSF for waiving of all charges for the computing time allocation.

Any other relevant information (if any): NONE

Title of ithe work carried out:

1. The electronic and optical properties of monovalent atom doped ZnO monolayers : the density functional theory.

2. Investigating structural, electronic, magnetic and optical properties of functionalized carbon nitride monolayer using density functional theory.

3. Theoretical study of structural, electronic, magnetic, and optical properties of core-shell magnetic nanoclusters.- under review

4. The Structural, Electronic And Optical Properties Of In- doped ZnO Monolayer : A First Principles Study - under review

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

E-mail Id: d_mrinal@yahoo.com

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

Name of the M. Phil/Ph. D. Students using NPSF

Sandhya Wakhare (Ph. D. Student), sandhya.wakhare@yahoo.co.in
Deepali Potekar (M. Phil. Student), deepalilohagaonkar@yahoo.com
Swapnil Deshpande (Ph. D. Student), d.swap9007@gmail.com

Research Challenge/s:

To calculate structural, electronic, magnetic, and optical, properties at atomic scale. It is challenging to calculate the bio-molecular sensing properties.

Work carried, Milestone, Achievements & Graphs, Plots:

1. The electronic and optical properties of monovalent atom doped ZnO monolayers: the density functional theory. ZnO nanosheet may be used as an alternative functional material as a pn homo junction. In view of the novel 2D character of the ZnO monolayer. A comparative study of different effects of alkali elements on structural and optical properties of ZnO monolayer can lead to better understanding of these materials as acceptors in ZnO structures. Such knowledge can enhance development of ZnO nanostructure-based optoelectronics devices. Using DFT, we have investigated the doping effects of alkali (Li, Na and K) elements on the structural, electronic and optical properties of a ZnO monolayer.

2. Investigating structural, electronic, magnetic and optical properties of functionalized carbon nitride monolayer using density functional theory. The understanding of structural, electronic, magnetic and optical properties of functionalized nanosheets for the applications like optoelectronic devices, sensors, device fabrication is an essential. We are basically working on the sensing properties of the graphene based materials. Among relevant investigations, the potential applications of graphene has been extensively studied earlier.

Normally pristine two dimensional materials sometimes cannot meet the demand of practical applications and hence functionalization is necessary to some extent. Now based on earlier studies, our interest is to study interaction of the functionalized graphene based two dimensional (2D) materials with toxic gas molecules in presence water or some solvents. We are interested to study the various properties of various phases of Nitrogen doped graphene, graphitic carbon nitride. We are also interested to study transport properties of these systems. These studies will be helpful for the improvement of selectivity sensitivity of the graphene based gas sensors. It will provide strong base for the experimental activities as well.

A detailed understanding of the interactions between bio-molecules and 2D nanomaterials surfaces is critical for the development of biomedical applications. Significance of 2D materials in bio-medicine is less clear at the present time. The creation of novel science in relation to bio- medicine and 2D materials is of immense importance, but the translation of these exciting developments into actual manufacturing is also crucial in order to facilitate applications. We are interested to understand role of graphene based materials as a biosensor considering interactions with the bio-molecules such as DNA, RNA and so on.

3. Theoretical study of structural, electronic, magnetic, and optical properties of core-shell magnetic nanoclusters.

The understanding of structural, electronic, magnetic and optical properties of magnetic core and effect of shelling over it by suitable bio compatible materials for biomedical applications is an essential. We are basically working on the interaction mechanism of the iron oxide as a core and effect of shelling by semiconducting nanoclusters. Based on the properties of core@shell clusters, we are interested to study its interaction with some bio-molecules. We hope that this project will provide theoretical support to the experimentalists for the development of the semiconducting devices and sensors.

Challenges : The computational investigations that we carry out in materials modeling & simulation study mostly deal with substantially large system size, which typically contains 1000 electrons. Hence, in order to model the electronic structure calculations, one always requires high performance computing facility equipped with efficient supercomputing resources. Further, depending on the nature and complexity of the properties (electronic, optical, magnetic, transport) to be determined, the required computing time is varied. The typical runtime for calculations of a complex atomic structure in our theoretical study is around 100 Hrs.

Publications / Articles etc. (If any):

1. S. Y. Wakhare, M. D. Deshpande, The electronic and optical properties of monovalent atom-doped ZnO monolayers: the density functional theory, Bulletin of Mater. Sci. 42 (5), 206, (2019).

2. S. S. Deshpande, M. D. Deshpande, T. Hussain and R. Ahuja, Investigating CO2 storage properties of C2N monolayer functionalized with small metal clusters, J. CO2 utilization, 35, (2020) 1-13. (Journal Impact Factor 5.189).

3. Manuscript by S. S. Deshpande, D. B. Potekar, M. D. Deshpande, P. B. Shelke, on Theoretical study of interaction of Fe13O8@Zn48O48 cluster with dopamine : Magnetic and optical properties submitted to J. Mol. Graph. Mod.

Awards (If any):

1. **Best poster** presentation on Magnetic and optical properties of Fe13O8@Zn48X48, (X = O, S, Se) core@shell clusters : Density Functional Theory Study at ICANN 2019, Palghar presented by Deepali Potekar.

2. **Best Poster** presentation on The structural, electronic and optical properties of functionalized GaN using DFT in Nanotsav, conference cum workshop on Nano-Science and Nanotechnology, organized at Sandip University in October 2019 presented by Sandhya Wakhare.

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

1. **Sandhya Wakhare** presented poster in ETMN-2019, International conference held at the Electronics Department, SPPU, Pune in Dec. 2019.

2. **Swapnil Deshpande** attended workshop on In silico quantum modelling studies at IUAC, New Delhi from 25th Nov. to 29th Nov. 2019.

3. **Deepali Potekar** participated and presented poster in International Conference on Advanced Nanomaterials Nanotechnology. (ICANN- 2019) at S. D. Arts, V. S. A. Commerce & M. H. M. Science College, Palghar from 26th to 28th November.

4. **Deepali Potekar** participated and presented poster at Dept. of Physics, Sandip University, Nashik from 11th to 12th October 2019.

5. **Sandhya Wakhare** presented poster in International conference, Nanotsav, Sandip university, Nashik in Oct. 2019.

6. **Sandhya Wakhare** presented poster at the RAMAN conference held at SPPU, Pune in Feb. 2019.

Felicitation Ceremony of the workshop "In silico quantum modelling studies" at IUAC, New Delhi.

Appreciation / Recognition (if any): Nil

References: Nil

Benefits & experience of using NPSF:

NPSF has been found very useful for us to carry out our scientific work.

Any other relevant information (if any): Nil

Title of the work carried out: Descriptors to predict dye-sensitized semiconductor based photocatalyst for hydrogen evolution reaction

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

Name and Email address of Research student: Subrahmanyam Sappati, subrahmanyamsappati@gmail.com

E-mail Id: prasenjit.jnc@gmail.com

Institution Name: IISER Pune

Research Challenge/s:

Discovering efficient photocatalysts for hydrogen production from water splitting is highly desirable. Usually most of the catalysts are discovered by a trial and error method. Computational studies can help in rational designing of such catalysts through high throughput screening of materials. However, for quick and efficient screening of materials one needs to identify descriptors that not only connects material properties with their functionality but are easy and inexpensive to compute.

Work carried , Milestone, Achievements & Graphs, Plots:

In this work we have tried to identify descriptors that can be used for computational predicting of photocatalysts for hydrogen evolution reaction. Using a combination of density functional theory based calculations and experiments we have studied the photocatalytic performance of ZnO nanoparticle and azo and thiophene based dyes to propose two descriptors, namely, charge injection efficiency and electron hole separation, that can be used for in silico design of new and efficient dye-sensitized-semiconductor composites as catalysts for hydrogen evolution reaction. The figure given below summarizes our work.

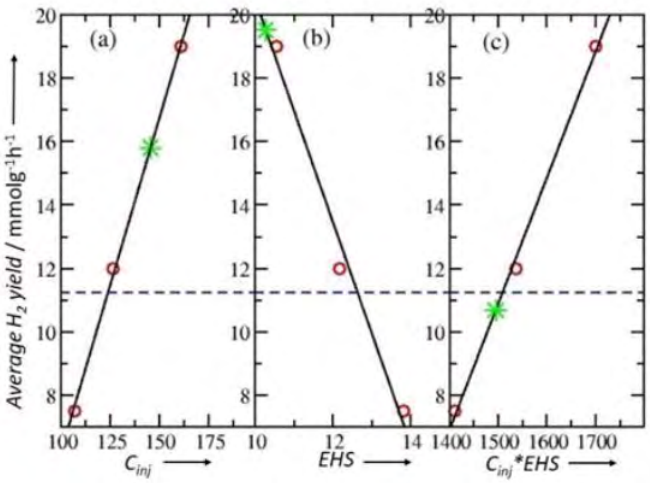


Fig. 1: Average H2 yield (AHY) in the reaction plotted against a) charge injection (C_{inj}), b) electron hole separation (*EHS*) (Å), c) product of C_{inj} and *EHS*. The symbols represent the actual data points while the black solid lines represent the fitted curve from azo dye composites. Blue dashed line (green star) denotes the experimental (predicted) AHY for T3′-Br.

Publications / Articles etc. (If any):

1. S. Sappati, L. George, V. P. Swami, R. Nandini Devi, and P. Ghosh, ChemCatChem., 11, 6460 (2019)

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:

We needed to perform several calculations for large systems, in particular to screen the thioophene dyes that would not have been possible without the usage of this facility.

Any other relevant information (if any): NA

Title of the work carried out: Hydrogen adsorption patterns on graphene supported on transition metal substrates

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

Name and Email address of Research student: Niharika Joshi, niharika.joshi@students.iiserpune.ac.in

E-mail Id: prasenjit.jnc@gmail.com

Institution Name: IISER Pune

Research Challenge/s:

Modification of graphene on transition metal support is perceived as an important way to tune the properties of graphene. However, the properties of the chemically modified semihydrogenated graphene depends on the H adsorption pattern, which is not easily discernible from experiments.

Work carried, Milestone, Achievements & Graphs, Plots:

In this work, using density functional theory based calculations, we have studied H adsorption patterns in graphene supported on lattice matched (111) surfaces of Ni, Co and Cu. We have considered uniform, arm-chair, zigzag and rectangular H patterns and found that all are equally probable on the supported graphene sheet. Our computation of the C-1s core-level X-ray photoemission spectra shows that the separation between the electron binding energies between different adsorption pattern are much smaller compared to the experimental resolutions.

Publications / Articles etc. (If any): N. Joshi and P. Ghosh, J. Ind. Chem. Soc., 96, 993 (2019) (Special Issue on Theoretical and Computational Chemistry)

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:

The computation of the core level spectra for so many configurations was very expensive and access to the NPSF facility made it possible for us to perform these calculations.

Any other relevant information (if any): NA

Title of the work carried out: First principles investigation of growth of small Pd-Ga bimetallic clusters on MgO(100) surface

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

Name and Email address of Research student: Nandha Kumar, nandha.kumar@students.iiserpune.ac.in

E-mail Id: prasenjit.jnc@gmail.com

Institution Name: IISER Pune

Research Challenge/s:

In most catalytic reactions small (a few atoms) clusters on the support are usually the active ones. However, at high reaction temperatures clusters may sinter or ripen to form larger clusters because of which the performance of the catalyst is detoriated. To prevent the sintering, it is important to understand the growth and sintering mechanisms of these clusters. Experimental study is quite challenging because it is difficult to control the different parameters. Computational studies require multi-scale modelling because of the time scales associated with these processes. Also one needs to take into account all the diffusion processes that makes modeling of these systems challenging and computationally expensive.

Work carried , Milestone, Achievements & Graphs, Plots:

Adsorption and diffusion of small sized PdGa bimetallic clusters on the MgO(100) surface are studied by density functional theory, and the growth mechanism of these bimetallic clusters is studied by graph- theoretical kinetic Monte Carlo simulations. All the pure clusters except Ga tetramers are found to be mobile on the surface, and the slow kinetics of Ga tetramers is attributed to its planar shape. At 300 K, all these clusters are kinetically stable and the vacancy sites act as the trapping centers. Upon increasing the temperature, Ga2, Ga3, and Pd1Ga2 clusters tend to escape from the vacancy sites rather than decomposing, whereas all other clusters tend to decompose. The growth of the pure Pd and Ga clusters is heterogeneous, though the elementary reactions involved in the growth process for these two clusters are very different. For the bimetallic PdGa clusters, our simulations show that the thermodynamically more stable Pd adatoms trapped at the vacancy site act as nucleation centers for the cluster growth, and the freely mobile Ga adatoms significantly influence the kinetics of cluster formation. When bimetallic clusters are grown by depositing Pd and Ga adatoms with an equal deposition rate, the bimetallic clusters are formed in the large proportion, especially the clusters with 1:1 atomic ratio are found in the highest fraction. Further, the clusters with the desired stoichiometric ratios can be obtained in a large fraction by varying the deposition rates of the Pd and Ga adatoms on the surface.

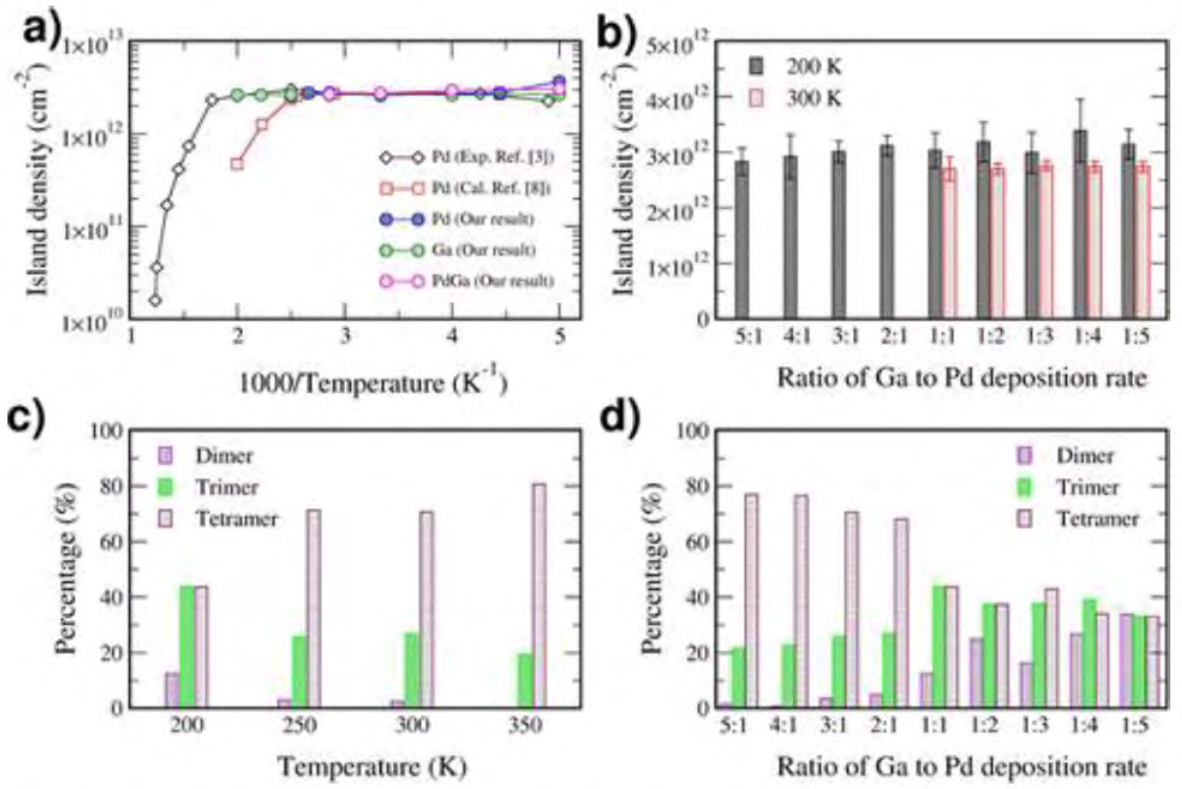


Fig. 1: (a) Estimated island density for the Pd, Ga, and PdGa clusters. (b) Estimated island density for the various ratios of Ga to Pd deposition rate at 200 and 300 K. (c) Size distribution of island density for the PdGa clusters grown at 200, 250, 300, and 350 K. (d) Size distribution of island density for the various ratios of Ga to Pd deposition rate at 300 K.

Publications / Articles etc. (If any):

N. Kumar, D. Chattaraj, I. Kaul, C. Majumdar, and P. Ghosh, J. App. Phys, 125, 185304 (2019).

Awards (If any): -

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

Appreciation / Recognition (if any): -

Benefits & experience of using NPSF:

For this project we needed to run about 300 nudged elastic band calculations to compute the diffusion barriers of the clusters that are inputs for our Kinetic Monte Carlo simulations. These calculations are parallelizable and hence using NPSF facility helped in speeding up the computations.

Any other relevant information (if any):

Title of the work carried out: Spontaneous and frequent conformational transitions provide a clue for the reaction chemistry between A...A mismatch in d(CAA.TAG) and mismatch repair proteins

Name & Designation of the Chief Investigator: Thenmalarchelvi Rathinavelan

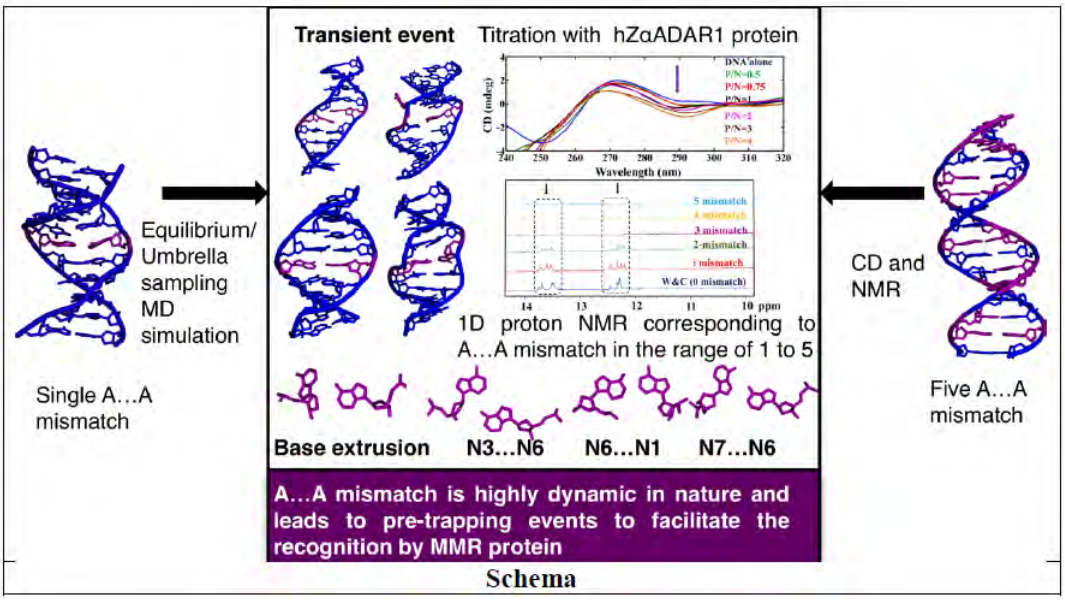
E-mail Id: tr@iith.ac.in

Institution Name: Indian institute of Technology Hyderabad.

Research Challenge/s:

Base pair mismatches can erroneously be incorporated in the DNA during replication and recombination etc. Here, the influence of A...A mismatch in d(CAA.TAG) is explored using molecular dynamics(MD) simulation, umbrella sampling simulation, circular dichroism(CD) and NMR techniques. MD simulations reveal that A...A mismatch experiences several transient events such as base flipping, base extrusion, etc., facilitating B-Z junction formation. A...A mismatch may assume such conformational transitions to circumvent the effect of nonisostericity with the flanking canonical base pairs so as to get accommodated in the DNA. CD and 1D proton NMR experiments further reveal that the extent of B-Z junction increases when the number of A...A mismatch in d(CAA.TAG)n=1-to-5 increases. CD titration studies of d(CAA.TAG)n=5 with the Z- DNA binding domain of human-ADAR1 protein show passive binding mode between the two, wherein, the binding of protein commences with B-Z junction recognition. Umbrella sampling simulation indicates that mismatch samples anti...+syn/+syn...anti, anti...anti +syn...+syn glycosyl conformations. The concomitant spontaneous transitions are: a variety of hydrogen bonding patterns, stacking and minor or major groove extrahelical movements (with and without the engagement of hydrogen bonds) involving adenines. These transitions frequently happen in anti...anti region compared to the other three regions as revealed from the lifetime of these states. Further, 2D-NOESY experiments indicate that the number of cross-peaks diminish with the increasing number of A...A mismatch implying its dynamic nature. The spontaneous extrahelical movement in A...A mismatch may be a key pre-trapping event in the mismatch repair as it drives the bases accessible to the sophisticated repair proteins.

Work carried, Milestone, Achievements & Graphs, Plots:



Publications / Articles etc. (If any): NA

Awards (If any):

BIRAC SRISTI - Gandhian Young Technological Innovation (GYTI) Award 2019 Winner

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

Appreciation / Recognition (if any): NA

References: NA

Benefits experience of using NPSF:

For longer simulation it is very much compatible because of higher configuration.
Data is very much safe.
Time saving.

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

Number of Ph.D scholars in 2019 who have used NPSF PARAM Yuva II (Information to be provided by CI of the project) : 02

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 is also investigated. Supersonic flow inside intakes and nozzles is also studied.

Work carried , Milestone, Achievements & Graphs, Plots:

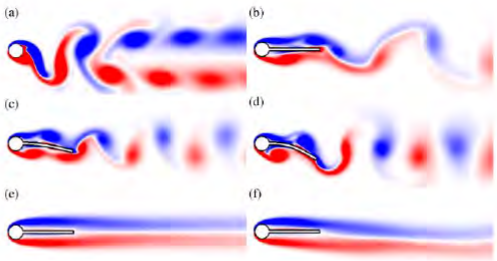


Figure 1. $Re = 150$, $m^* = 10$, flow past an elastically mounted cylinder with and without plate: instantaneous vorticity field for (a) $U_s^* = 5$, isolated cylinder, (b) $(U_s^*, U_p^*) = (6, 0)$, (c) $(U_s^*, U_p^*) = (5.5, 7.4)$, (d) $(U_s^*, U_p^*) = (6.0, 12.8)$, (e) $(U_s^*, U_p^*) = (12, 0)$, and (f) $(U_s^*, U_p^*) = (16.5, 0)$ when the cylinder displacement is at maximum location. (a-d), (e) and (f) are for VIV regime at peak amplitude of cylinder response, steady flow and galloping response, respectively.

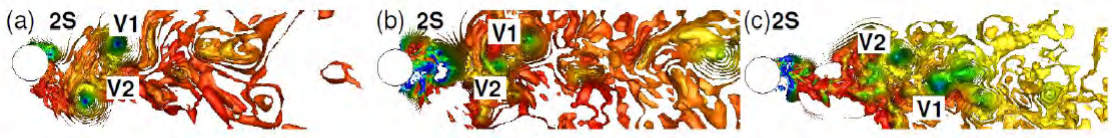


Figure 2. $U^* = 5.0$, $3D$ –VIV of a cylinder: Instantaneous pressure iso-contours (a) $Re = 5.0 \times 10^4$ (b) $Re = 1.5 \times 10^5$and (c) $Re = 3.0 \times 10^5$ at an instant when the displacement of the cylinder is at its maximum position.

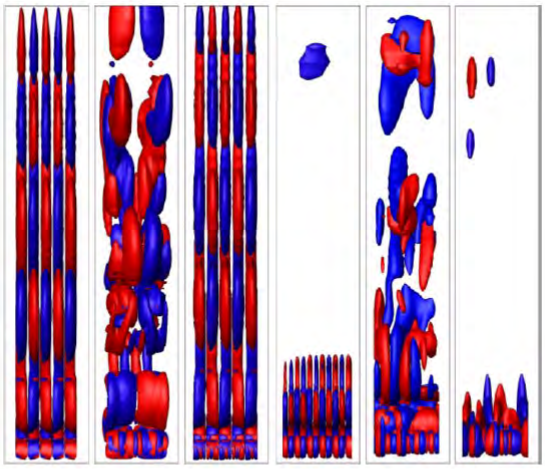


Figure 3. $Re = 200, 3D$ –VIV of a rotating cylinder: instantaneous spanwise vorticity iso-surface for $(\alpha = 1.5, U^* = 6.5, (b)\alpha = 1.5, U^* = 9.5, (c)\ \alpha = 1.8, U^* = 6.5, (d)\ \alpha = 1.8, U^* = 9.5\ (e)\alpha = 2.5, U^* = 8$ and $(f)\alpha = 2.5, U^* = 30.0$, when the cylinder displacement is maximum.

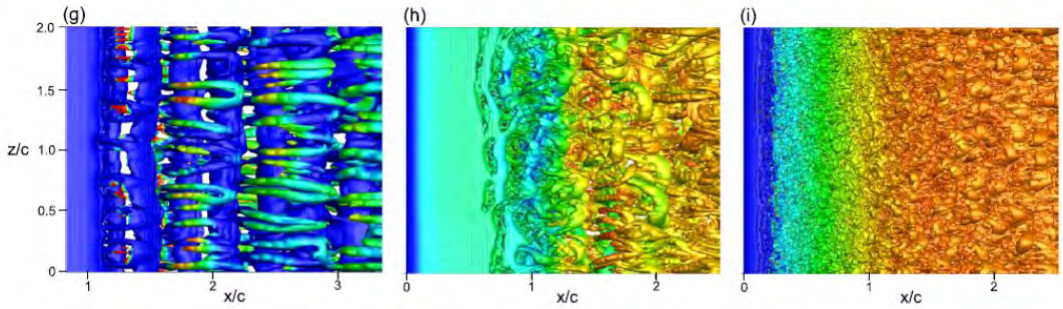


Figure 4. $\alpha = 10^0$, 3D flow past an Eppler 61 airfoil: instantaneous Q isosurface colored with the coefficient of pressure for $(g)\ Re = 4000, (h)Re = 15\,000$ and $(i)Re = 38000$.

Publications / Articles etc. (If any):

1. Journal of Fluid Mechanics (3.137)
   Tulsi Ram Sahu, Mohd Furquan, Sanjay Mittal, "Numerical study of flow-induced vibration of a circular cylinder with attached flexible splitter plate at low Re, Journal of Fluid Mechanics, 880, 551-593 (2019).

2. Physics of Fluids (2.627)
   Samuthira Pandi Jawahar Sivabharathy, Sanjay Mittal, "Wake transitions and laminar separation bubble in the flow past an Eppler 61 airfoil, Physics of Fluids, 31(11), 114102 (2019).

3. Journal of Fluids and Structures (3.070)
   Tulsi Ram Sahu, Mohd Furquan, Yash Jaiswal, Sanjay Mittal, "Flow-induced vibration of a circular cylinder with rigid splitter plate", Journal of Fluids and Structures, 89, 244-256 (2019).

4. Journal of Fluid Mechanics (3.137)
   Navrose, Sanjay Mittal, Intermittency in free vibration of a cylinder beyond the laminar regime, Journal of Fluid Mechanics, 870, R2.1-14 (2019).

5. Physics of Fluids (2.627)
   Kunjal Shah, Ravi Shakya, Sanjay Mittal, "Aerodynamic forces on projectiles used in various sports", Physics of Fluids, 31, 015106 (2019).

6. Physics of Fluids (2.627)
   Gaurav Chopra, Sanjay Mittal, Drag coefficient and formation length at the onset of vortex shedding, Physics of Fluids, 31(1), 013601 (2019).

Awards (If any): NA

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

1.Gaurav Chopra, Sanjay Mittal, Vortex formation length near the onset of vortex shedding in flow past a circular cylinder, Asian congress of Fluid Mechanics (2019), JNCASR Bengaluru, India.

Figure 5.4: Mr. Gaurav Chopra (PhD student) during oral presentation in Asian congress of Fluid Mechanics held at the Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India

2.Tulsi Ram Sahu, Mohd Furquan, Sanjay Mittal, Computational study of flow-induced vibration of a circular cylinder with flexible splitter, Asian congress of Fluid Mechanics (2019), JNCASR Bengaluru, India.

Figure 5.5: Mr. Tulsi Ram Sahu (PhD student) during poster presentation in Asian congress of Fluid Mechanics held at the Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India

3.Tulsi Ram Sahu, Gaurav Chopra, Sanjay Mittal, Vortex-induced vibration of a circular cylinder at high Reynolds number, Symposium on Fluid-Structure-Sound Interactions and Control (2019), Chania, Crete island, Greece.

Appreciation / Recognition (if any):

References:

Benefits & experience of using NPSF: NA

Any other relevant information (if any):

Title of the work carried out: Decaying turbulence and magnetic fields in galaxy clusters

Name & Designation of the Chief Investigator: Sharanya Sur, Reader

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

Institution Name: Indian Institute of Astrophysics

Research Challenge/s:

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

Free decay of magnetohydrodynamic (MHD) turbulence has been an active area of research in a variety of contexts. Starting from the generation of largescale primordial magnetic fields in the early Universe, decaying MHD turbulence has also been studied in connection with the recent detection of strong optical polarization in gammaray burst (GRB) afterglows and to measure the decay rates of sub- and super-Alfvenic supersonic turbulence in the interstellar medium. A common feature in these works is that they all start from a magnetically dominated regime with the field initialized by a power spectrum peaked at around a large wavenumber. In galaxies and clusters the magnetic Reynolds numbers (Rm) are large enough to excite a Fluctuation/small-scale dynamo. The resulting field exhibits an intermiWent structure with the magnetic energy spectrum peaked at resistive scales at early times which then gradually shifts to larger scales as the dynamo approaches saturation. Using a part of the computing time at Param Yuva II, we explored the decay of turbulence and such dynamo generated fields in the context of galaxy clusters where such a decaying phase can occur in the aftermath of a major merger event. Irrespective of the compressibility of the flow, we found that both rms velocity and magnetic field decay as a power-law in time. In the subsonic case we find that the exponent of the power-law is consistent with the $-3/5$ scaling reported in previous studies. However, in the transonic regime both the rms velocity and the magnetic field initially undergo rapid decay with an ˆ1.1 scaling with time. This is followed by a phase of slow decay where the rms velocity exhibits an 3/5 scaling in time while the rms magnetic field scales as 5/7. Furthermore, analysis of the Faraday rotation measure reveals that the Faraday RM decays also decays as a power law in time ˆ5/7; steeper than the ˆ2/5 scaling obtained in previous simulations of magnetic field decay in subsonic turbulence.

Publications / Articles etc. (If any):

Title: Decaying turbulence and magnetic fields in galaxy clusters , Journal: Monthly Notice of the Royal Astronomical Society, Vol 488, Issue 3, Pages : 34393445, 2019. Journal Impact factor: 5.231

Awards (If any):

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

a) Conference on Plasma Simulations, 2324th Jan.2020, Institute for Plasma Research, Gandhinagar

Appreciation / Recognition (if any): NA

References:

Benefits & experience of using NPSF:

Any other relevant information (if any):

Title of the work carried out: Strain induced Band structure tuning in SnS2 monolayers

Name & Designation of the Chief Investigator: Dr.Sriprakash G, Associate professor, Maharani cluster University, Bangalore-560001

E-mail Id: sriprakash72@gmail.com

Institution Name: Department of Physics, Maharani Cluster University, Bangalore-560001

Research Challenge/s:

The computational work started from December-2019.

Work carried , Milestone, Achievements Graphs, Plots:

The band structure calculations are carried out in quantum espresso for different strains and band structures show variation in band gap. The wave- functions determined from these calculations are further processed in yambo - many body codes. Results need to be analyzed.

Publications / Articles etc. (If any): The articles regarding the above mentioned work will be Communicated once the complete calculations are validated.

Awards (If any): -

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

Appreciation / Recognition (if any): -

References: -

Benefits & experience of using NPSF:

I have found quantum espresso highly useful. But abinit is not working to my expectations.

Any other relevant information (if any):

Title of the work carried out: Conformational Dynamics of Intrinsically Disordered and Ordered Protein

Name & Designation of the Chief Investigator: Dr. Sunita Patel (DST Women Scientist)

Student: Akhil Sudarsan (8th semester, CEBS) Email: akhil.sudarsan@cbs.ac.in

E-mail Id: sunita.patel@cbs.ac.in

Institution Name: UM-DAE Centre for Excellence in Basic Sciences, Mumbai

Research Challenge/s:

There have been several challenges in studying intrinsically disordered proteins (IDPs). Since these proteins are devoid of definite structure achieving conformational convergence in molecular simulation is a great problem. This is a subjective challenge. Besides, we have other set of problems such as supercomputer down time, a long job queue and connectivity problem due to network problem which together pose a big challenge in completing the project.

Work carried , Milestone, Achievements & Graphs, Plots:

Crystallin proteins are ubiquitous in nature. They are found in almost all life forms. Although, they are ubiquitous in nature, prevalence is observed in the vertebrate eye lens. Cataract is caused due to opacity in the eye lens. Blindness due to cataract constitutes 48% of the world population. Most of the crystallin proteins are highly ordered and are well known for their high structural stability. The primitive archaeal and microbial crystallins are stabilized further by binding to Ca2+. However, several eye-len crystallins impart higher stability without Ca2+. There are distinct regions in the crystallin domain responsible for its unusual stability. Mutation(s) in these regions cause local and/or global change in the structure which in turn could promote aggregation. A number of studies showed a direct connection between partial or complete structural unfolding and aggregation. It is important to identify such regions on the crystallin domain to understand aggregation related disease such as cataract.

In this study, we characterized, the partially folded or unfolded structures of M-crystallin which are resulted due to site specific mutations. This protein is having similar structure like that of eye-lens crystallin, so the mutational studied carried out here can be extended to derive conclusions on the eye- lens crystallin. M-crystallin is mutated in the hydrophobic core and/or in two Ca2+ binding sides based on the sequence alignment with the intrinsically disordered, Hahellin and highly ordered eye-lens D- crystallin. The mutant shows more number of distinct clusters indicating various unfolded conformations (Figure 1). These unfolded conformations has exposed solvent accessible surface area which is responsible for the aggregation of the mutant protein. This study provides, mechanistic insight of conformational transition from an ordered to disordered states. Thus, it provides a rational to the cause of aggregation.

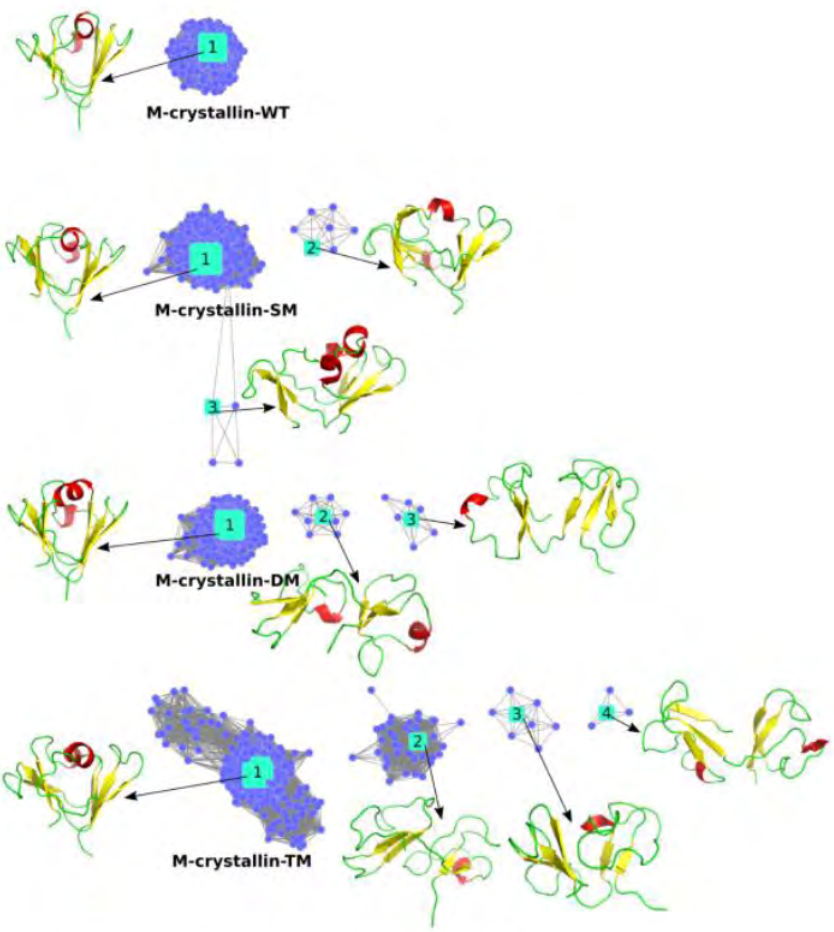


Figure 1. Network cluster analysis. Pairwise RMSD cutoff is 5 Å.

Publications / Articles etc. (If any):

Patel S.*, Krishnan B., Hosur R.V., Chary K.V.R. (2019) Mechanistic Insights from Replica Exchange Molecular Dynamics Simulations into Mutation Induced Disordered-to-Ordered Transition in Hahellin, a -Crystallin. J Phys Chem B. 123:5086-5098. (* Corresponding author), PMID- 31136713; IF-2.9, ISSN: 1520-6106 (print); 1520-5207 (web).

Awards (If any):

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

The work presented in following two conferences. Two pictures of the presentation held at TIFR Mumbai are given below.

1. (Oral speaker) "Mechanistic insights into mutation induced conformational transition from disordered-to-ordered state in Hahellin, a -crystallin" in the International conference on Multiscale Simulation Mathematical Modelling of Complex Biological System held in Jawaharlal Nehru University from Jan 30 to Feb 01, 2019.

2. (Oral speaker) Mutation induced conformational transition from disordered-to-ordered state in a - crystallin, Hahellin in an one-day symposium on NMR in Biological System held at Tata Institute of Fundamental Research Mumbai on April 27, 2019.

Appreciation / Recognition (if any):

References:

Professor, V.K. Jain, Department of Chemistry, UM-DAE Center for Excellence in Basic Sciences, Kalina, Mumbai - 400 098, INDIA. Phone: 02226524989 E-mail: jainvk@cbs.ac.in

Senior Professor (retired), R. V. Hosur, Department of Chemistry, UM-DAE Center for Excellence in Basic Sciences, Kalina, Mumbai - 400 098, INDIA.and Chemical Sciences, TIFR Mumbai, Colaba, Mumbai - 400005, INDIA Phone: 9987051556 Email: rvhosur53@gmail.com

Benefits & experience of using NPSF:

We are deprived of supercomputing facility in our institution. Having NPSF is a great support to boost our research. The computational facility available at NPSF although is not sufficient it is better than none situation for us. Therefore, it is serving as a great support system to carry out our computational research work.

Any other relevant information (if any):

Title of the work carried out: Quasiparticle band gap, vibrational and transport properties of one and two-dimensional nanosystems.

Name & Designation of the Chief Investigator: Dr. Utpal Sarkar, Assistant Professor, Department of Physics Assam University, Silchar

E-mail Id: utpalchemiitkgp@yahoo.com; utpalchemiitkgp@gmail.com

Institution Name: Assam University, Silchar

Research Challenge/s:

Even though DFT is a very useful tool in predicting the ground state properties for most systems, it is unable to address some specific fundamental phenomena in strongly correlated systems. In such situations, it is necessary to go beyond ground-state theory. Using Green's function based many-body approaches such as G0W0 based on a fixed reference, self-consistent GW approaches (for predicting the correct band gap), the Bethe-Salpeter equation it is possible to study neutral excitations (e.g., for optical properties). For calculating GW band gap and optical response with Bethe-Salpeter equation (BSE) approach, it requires much computational resources, which is the main challenging part.

Work carried , Milestone, Achievements & Graphs, Plots:

Work carried: Using the NPSF resources we have studied electronic and optical properties of newly designed graphyne with XN at hexagonal ring (labeled as XN-ynes, where X = B, Al, Ga) and graphyne with BP at hexagonal ring (labeled as BP-yne). We have calculated GW corrected band gap for all these systems. Except for BN-yne and BP-yne, all other XN-ynes are indirect band gap semiconductors, having a larger gap than pristine graphyne. The phonon dispersion curves are determined for all these structures to check the dynamic stability of all these systems. Optical response with Bethe-Salpeter equation (BSE) approach have also been determined for all these materials. The strong absorption peak for XN-ynes lies in UV region of electromagnetic spectra also suggesting their possible use as UV light absorber whereas the optical band gap, as well as the strong absorption peak, lies in the near-infrared region (NIR) for BP-yne and this promising trait can be exploited in biomedical arena.

Achievements: We have published two papers based on the work done using NPSF resources.

Publications / Articles etc. (If any):

1. Barnali Bhattacharya, Jyotirmoy Deb, Utpal Sarkar, "Boron-phosphorous doped graphyne: A near-infrared light absorber", AIP Advances, 9, 095031 (2019).
2. Barnali Bhattacharya, Debolina Paul, Utpal Sarkar, Electronic and optical properties of XN-ynes (X = B, Al, Ga): A first-principle study with many-body effects, Applied Surface Science, 495, 143612 (2019).

Awards (If any): Selected as a member of The National Academy of Sciences India (NASI) (Nomination basis).

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

Appreciation / Recognition (if any): Selected as a member of The National Academy of Sciences India (NASI) (Nomination basis).

References: NA

Benefits & experience of using NPSF:

Using NPSF resources we have studied some fundamental phenomena in strongly correlated systems for which much higher computational resources is required. We have also published our results in journals of international repute.

Any other relevant information (if any):

Title of the work carried out: Hypersonic Flow and Heat Transfer

Name of the Application Research Field of the project: Computational Fluid Dynamics

Name & Designation of the Chief Investigator: Dr. Ashoke De, Associate Professor, Dept. of Aerospace Engineering, IIT Kanpur, 208016, India

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

Institution Name: Indian Institute of Technology Kanpur, India

Name and Email address of the researchers/students: Mr. Gaurav Kumar, Dept. of Aerospace Engineering, IIT Kanpur, 208016, India. Email: gauravkr@iitk.ac.in

Information of the Ph.D scholars who have completed Ph.D in 2019: None

Number of Ph.D scholars in 2019 who have used NPSF PARAM Yuva II system: 02

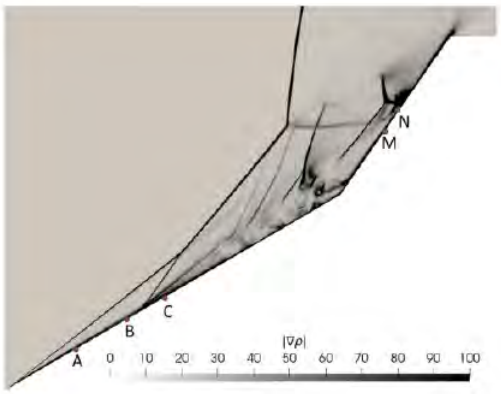
Research Challenge/s:

The hypersonic flow over a double wedge configuration is mostly influenced by the unsteady shock-shock, shock-boundary layer and shock-separation region interaction. The overall flow structure comprises shocks, vortices, separation region and shear layers. Their interaction with each other affects the distribution of surface heat transfer rates. The impingement of shock waves on the wall results in very high peak values in the surface heat fluxes and an accurate prediction of the location and peak values of such surface heat fluxes is a big challenge.

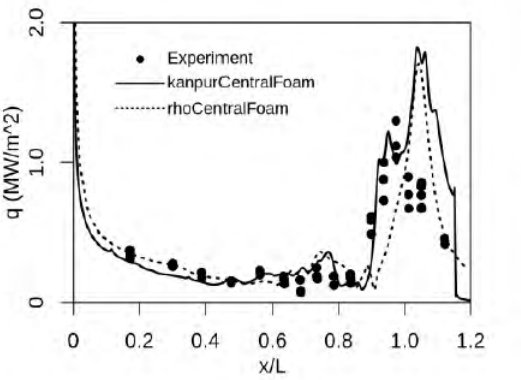
Work carried / Milestone / Achievements:

A new high fidelity open-source CFD program has been created in OpenFOAM [1] framework to simulate hypersonic flows for prediction of extremely high heat transfer rates on solid surface corners. This new program is named kanpurCentralFoam after its predecessor rhoCentralFoam and since it has been developed at IIT Kanpur. This solver is, numerically, much more accurate and efficient compared to its predecessor and in terms of computational efficiency, this new program generated is highly scalable over a large number of nodes. New solutions obtained using NPSF compute nodes are under post-processing and analysis process. A few preliminary results are shown in figure below.

Fig (a) shows the plot of density gradient for a hypersonic flow at Mach number 7 over a double wedge configuration. A very accurate prediction of shock patterns is observed compared to the previous experimental results [2]. Fig (b) shows the comparison of new simulation using our solver kanpurCentralFoam, results published with previous solver rhoCentralFoam [3] and previously published experimental results [2]. New results obtained in our computation have significant improvement compared to previously published numerical results.



(a)



(b)

Publications / Articles etc. (If any):

An improved density based compressible flow solver in OpenFOAM for unsteady flow calculations. Submitted to Computer and Mathematics with applications Dec 29, 2019

Awards (If any): NA

References:

1. Greenshields, C.J., 2015. Openfoam user guide. OpenFOAM Foundation Ltd, version, 3(1), p.47.

2. Swantek, A., 2012. The role of aerothermochemistry in double cone and double wedge flows (Doctoral dissertation, University of Illinois at Urbana-Champaign). [3] Durna, A.S. and Celik, B., 2019. Time-periodic shock interaction mechanisms over double wedges at Mach 7. Shock Waves, 29(3), pp.381-399.

Benefits experience of using NPSF:

The computation facility provided NPSF has been very helpful in performing large scale computations and we are very grateful to CDAC for providing us this facility.

Any other relevant information (if any): NA

Title of the work carried out: There are three projects with the following titles:
a) Exploring the protein stability and flexibility by comparative molecular dynamics simulations of homologous Hyperthermophilic, Mesophilic, and Psychrophilic proteins.
b) Structure-based drug designing and molecular dynamics studies of Plasmepsins of Plasmodium Falciparum for malaria
c) Computational study for drug delivery using Metal-Organic Frameworks as a carrier

Name & Designation of the Chief Investigator: Malay Kumar Rana, Assistant Professor, Department of Chemical Sciences, Indian Institute of Science Education and Research Berhampur

E-mail Id: mrana@iiserbpr.ac.in

Institution Name: Indian Institute of Science Education and Research Berhampur

Research Challenge/s:

- Homologous (Hyperthermophilic, Mesophilic, and Psychrophilic) proteins adapted to different physiological conditions exhibit differences in their functions by modulating stability and flexibility. However, quantifying stability and flexibility of these proteins existing in different species under different physiological conditions has been yet to explore, which is objective of this project.
- Malaria is a life-threatening disease caused by plasmodium parasites and which is transmitted to humans through infected female Anopheles mosquitoes. The aim of the project is to perform structure-based drug designing to inhibit plasmodium parasites.
- Because of porous integrity and selective interactions, metal-organic frameworks are a suitable carrier for drug molecules for acute delivery to treat various cancers and other diseases. However, this is quite unexplored till date. Finding out the best carriers for drugs is an ultimate goal of this project.

Work carried , Milestone, Achievements Graphs, Plots: We received the approval on Dec 25, 2019. During Jan, 2019 Dec, 2019, each of respective work was just started.

Publications / Articles etc. (If any):

Awards (If any):

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

Appreciation / Recognition (if any):

References:

Benefits & experience of using NPSF:

We are very much grateful to C-DAC to permit to use the facility to carry out the above-mentioned projects. I do see their great support to overcome any technical hurdles faced at the time of utilization of the C-DAC computational facility.

Any other relevant information (if any):

I look forward to have a great experience with C-DAC. At the outset, I really appreciate the C-DAC staff for being very humble, prompt and efficient.

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5.2 Ph.D Theses

1. **Title of the thesis : ATOMIC-SCALE INSIGHTS INTO ENERGY CONVERSION IN TWO DIMENSIONAL TRANSITION METAL DICHALCOGENIDE MONOLAYERS FROM AB-INITIO STUDIES**
   Ph.D Scholar Name :Mr. Dimple Sharma
   Name of the Supervisor : Prof Abir De Sarkar
   Name of the Institute : Institute of Nano Science & Technology, Mohali

2. **Title of the thesis : NA**
   Ph.D Scholar Name: Ms. Tasneem Kausar
   Name of the Supervisor: Dr. Md. Shahid Nayeem
   Name of the Institute : Aligarh Muslim University, Aligarh

3. **Title of the thesis : THEORETICAL INVESTIGATION OF OPTICAL AND TRANSPORT PROPERTIES OF NANO-STRUCTURED SYSTEMS**
   Ph.D Scholar Name : Ms. Barnali Bhattacharya
   Name of the Supervisor: Dr. Utpal Sarkar
   Name of the Institute : Department of Physics, Assam University, Silchar

4. **Title of the thesis : Theoretical investigations on interactions among molecules, hydrogen bonded water clusters and their response to externally applied electric fields**
   Ph.D Scholar Name: Ms. Nalini Dattatraya Gurav
   Name of the Supervisor: Prof. Dr. Rajeev K. Pathak (co-guide: Prof. Dr. Shridhar P. Gejji)
   Name of the Institute: Department of Physics (and Chemistry), Savitribai Phule Pune University, Pune.

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5.3 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.

Publications 2019

Journal of Materials Chemistry A (10.73)

Manisha Das, Nityasagar Jena, Taniya Purkait, Navpreet Kamboj,Abir De Sarkar,0 Ramendra Sundar Dey, "Single-phase Ni5P4-Copper foam superhydrophilic and aerophobic core-shell nanostructures for efficient hydrogen evolution reaction", Journal of Materials Chemistry A,07, 23989-23999 (2019)

ACS Applied Materials & Interfaces (8.45)

Manish Kumar Mohanta, Ashima Rawat, Nityasagar Jena, Dimple, Raihan Ahammed, Abir De Sarkar*,"Interfacing boron monophosphide with molybdenum disulphide for an ultra-high performance in thermoelectrics, 2D excitonic solar cells and nanopiezotronics", ACS Applied Materials & Interfaces, 12, 3114-3126 (2020)

J. of Hazardous Materials (7.65)

Munish Shorie, Harmanjit Kaur, Gaganpreet Chadha, Kulvinder Singh, and Priyanka, Sabherwal Graphitic Carbon nitride QDs impregnated biocompatible agarose cartridge for removal of heavy metals from contaminated water samples. J. of Hazardous Materials 367, 629 (2019).

Nanoscale (6.97)

Manish Kumar Mohanta, Ashima Rawat, Dimple, Nityasagar Jena, Raihan Ahammed, Abir De Sarkar*, "Super high out-of-plane piezoelectricity, low thermal conductivity and photocatalytic abilities in ultrathin 2D van der Waals heterostructures of Boron Monophosphide and Gallium Nitride",Nanoscale, 11, 21880-21890 (2019)

Monthly Notice of the Royal Astronomical Society (5.231)

Sharanya Sur, Decaying turbulence and magnetic fields in galaxy clusters Journal: Monthly

Notice of the Royal Astronomical Society, Vol 488, Issue 3, Pages: 3439 - 3445, 2019.

J. CO2 utilization (5.189)

S. S. Deshpande, M. D. Deshpande, T. Hussain and R. Ahuja, Investigating CO2 storage properties of C2N monolayer functionalized with small metal clusters, J. CO2 utilization, 35, (2020) 1-13.

Applied Surface Science (5.15)

Gaganpreet, Enhanced sensitivity of band gap engineered phosphorene towards NH3 and NO2 toxic gases, Applied surface Science, 50, 144967 (2019).

Barnali Bhattacharya, Debolina Paul, Utpal Sarkar, Electronic and optical properties of XN-ynes (X = B, Al, Ga): A first-principle study with many-body effects, Applied Surface Science, 495, 143612 (2019).

Raihan Ahammed, Ashima Rawat, Nityasagar Jena, Dimple, Manish Kumar Mohanta, Abir De Sarkar*,"ZrS3/MS2 and ZrS3/MXY (M=Mo, W; X, Y=S, Se, Te; X00Y) type-II van der Waals hetero-bilayers: Prospective candidates in 2D excitonic solar cells", Applied Surface Science,499, 143894 (2020)

Taniya Purkait, Raihan Ahammed, Abir De Sarkar, Ramendra Sundar Dey, "The role of exfoliating solvents for control synthesis of few-layer graphene-like nanosheets in energy storage applications: Theoretical and experimental investigation", Applied Surface Science, 509 (2020) 145375

Inorganic Chemistry (4.85)

Alessia Provino, Volodymyr Smetana, Timothy A. Hackett, Durga Paudyal, Manish K. Kashyap, Cristina Bernini, Amitava Bhattacharyya, Sudesh K. Dhar, Marcella Pani, Flavio Gatti, Anja-Verena Mudring, and Pietro Manfrinetti, Stability, Crystal Chemistry, and Magnetism of U2+xNi21-xB6 and Nb3-yNi20+yB6 and the Role of Uranium in the Formation of the Quaternary U2-zNbzNi21B6 and UdNb3-dNi20B6 Systems, Inorg. Chem. 58, 15045-15059 (2019).

J. Mol. Liquids (4.561)

Tajalli Ilm Chandel, Aiman Masroor, Mohammad Khursheed Siddique, Ibrar Ahmad Siddique, Ishrat Jahan, Maroof Ali, Shahid M. Nayeem, Vladimir N. Uversky, Rizwan Hasan Khan, " Molecular basis of the inhibition and disaggregation of thermally-1 induced amyloid fibrils of human serum albumin by an anti-2 Parkinson's drug, benserazide hydrochloride" , J. Mol. Liquids, 275 (2019), 553-567.

Faisal Ameen, Sharmin Siddiqui, Ishrat Jahan, Shahid M. Nayeem, Sayeed Ur Rehman, Mohammad Tabish, " A detailed insights into the interaction of Memantine with bovine serum albumin: a spectroscopic and computational approach." J. Mol. Liquids (Accepted).

ChemCatChem (4.495)

S. Sappati, L. George, V. P. Swami, R. Nandini Devi, and P. Ghosh, Descriptors to Predict Dye-Sensitized Semiconductor Based Photocatalyst for Hydrogen Evolution Reaction ,ChemCatChem., 11, 6460 (2019)

Journal of Physical Chemistry C (4.31)

Ashima Rawat, Raihan Ahammed, Dimple Sharma, Nityasagar Jena, Manish Kumar Mohanta, Abir De Sarkar*, "Solar Energy Harvesting in Type II van der Waals Heterostructures of Semiconducting Group III Monochalcogenide Monolayers", Journal of Physical Chemistry C, 123, 12666-12675 (2019)

Krishnanjan Pramanik, Kartik Sau, P. Padma Kumar, "Role of Framework Flexibility in Ion Transport: A Molecular Dynamics Study of LiM2(PO)4", J. Phys. Chem. C 2020 (in Press). DOi:https://doi.org/10.1021/acs.jpcc.9b11624 [doi.org]

J. Alloys Compd (4.175)

AmitSonia, K.C.Bhamu, JagratiSahariya, Investigating effect of strain on electronic and optical properties of lead free double perovskite Cs2AgInCl6 solar cell compound: A first principle calculation; J. Alloys Compd. 817 (2020) 152758.

Journal of Physical Chemistry A (4.09)

Sumitra Godara, Manikandan Paranjothy, "Competing Molecular and Radical Pathways in the Dissociation of Halons via Direct Chemical Dynamics Simulation", J. Phys. Chem. A, 123, 8527-8535(2019)

Physical Review B (3.74)

Nityasagar Jena, Dimple,0Raihan Ahammed, Ashima Rawat, Manish Kumar Mohanta,0Abir De Sarkar*,"Valley drift and valley current modulation in a strained monolayer MoS2", Physical Review B 100, 165413 (2019)

Biophys. J (3.665)

Ishrat Jahan and Shahid M. Nayeem, Effect of osmolytes on conformational behaviour of intrinsically disordered protein -synuclein", Biophys. J., 2019, 117 (10), 1922-1934

Phys. Chem. Chem. Phys. (3.567)

Aarti Sindhu, Renuka Pradhan, Upakarasamy Lourderaj, Manikandan Paranjothy, " Theoretical investigation of the isomerization pathways of diazenes: torsion vs. inversion", Phys. Chem. Chem. Phys., 21, 15678-15685 (2019)

J. Cell. Biochem (3.448)

S. Shuaib, S. S. Narang, D. Goyal, B. Goyal, Computational design and evaluation of β-sheet breaker peptides for destabilizing Alzheimer's amyloid-β 42 protofibrils. J. Cell. Biochem. 2019, 120, 17935.

Bulletin of Mater. Sci. (3.442)

S. Y. Wakhare, M. D. Deshpande, The electronic and optical properties of monovalent atom-doped ZnO monolayers: the density functional theory, Bulletin of Mater. Sci. 42 (5), 206, (2019).

Nanotechnology (3.399)

Anjali Panwar, Vikas Malik, S Neeleshwar, Anjana Bagga*, Probing the path for achieving a broad temperature plateau of the figure of merit in thermoelectric nanocomposite materials, Nanotechnology 31 (3), 035405 (2019)

J. Biomol. Struct. Dyn.(3.31)

S.S.Narang, D. Goyal, B. Goyal, Inhibition of Alzheimer's $amyloid-\ \beta\ -42$ peptide aggregation by a $bi-$functional $bis-$tryptoline triazole: key insights from molecular dynamics simulations. J. Biomol. Struct. Dyn. 2019, doi.org/10.1080/07391102.2019.1614093.

Physica E: Low-dimensional Systems and Nanostructures (3.176)

Rajesh Thakur, P. K. Ahluwalia, Ashok Kumar, Brij Mohan, Raman Sharma. "Electronic Structure and Carrier Mobilities of Twisted Graphene Helix", [arxiv link: https://arxiv.org/abs/1909.05278]

Neha Katoch, Ashok Kumar, Raman Sharma, P. K. Ahluwalia and Jagdish Kumar Strain Tunable Schottky Barriers and Tunneling Characteristics of Borophene/MX2 van der Waals HeterostructuresPhysica E: Low-dimensional System and Nanostructures, 113842 (accepted and in press). https://doi.org/10.1016/j.physe.2019.113842

Journal of Fluid Mechanics (3.137)

Navrose, Sanjay Mittal, in free vibration of a cylinder beyond the laminar regime, Journal of Fluid Mechanics, 870, R2.1-14 (2019).

Tulsi Ram Sahu, Mohd Furquan, Sanjay Mittal, "Numerical study of flow-induced vibration of a circular cylinder with attached flexible splitter plate at low Re, Journal of Fluid Mechanics,880, 551-593 (2019).

Journal of Fluids and Structures (3.070)

Tulsi Ram Sahu, Mohd Furquan, Yash Jaiswal, Sanjay Mittal, "Flow-induced vibration of a circular cylinder with rigid splitter plate",0Journal of Fluids and Structures,89, 244-256 (2019).

New J. Chem (3.069)

Sharmin Siddiqui, Faisal Ameen, Ishrat Jahan, Shahid M. Nayeem and Mohammad Tabish, comprehensive spectroscopic and computational investigation on the binding of anti-asthmatic drug triamcinolone with serum albumin, New J. Chem., 2019, 43, 4137-4151

The Journal of Physical Chemistry B (3.00)

Patel S.*, Krishnan B., Hosur R.V., Chary K.V.R. (2019) Mechanistic Insights from Replica Exchange Molecular Dynamics Simulations into Mutation Induced Disordered-to-Ordered Transition in Hahellin, a $\beta\gamma$-Crystallin. J Phys Chem B. 123:5086-5098. (* Corresponding author), PMID- 31136713; IF-2.9, ISSN: 1520-6106 (print); 1520-5207 (web).

Vishwanath Reddy, Moumita Saharay, Solubility of Caffeine in Supercritical CO2: A Molecular Dynamics Simulation Study, The Journal of Physical Chemistry B, 2019, 123, 9685-9691

Journal of Physical Chemistry B (2.923)

Bappa Ghosh, Srabanti Chaudhury, "Translocation Dynamics of an Asymmetrically Charged Polymer through a Pore under the Influence of Different pH Conditions", J. Phys. Chem. B, 123, 4318-4323 (2019)

J. Phys. Chem. A (2.836)

Sumitra Godara, Manikandan Paranjothy, " Competing Molecular and Radical Pathways in the Dissociation of Halons via Direct Chemical Dynamics Simulation", J. Phys. Chem. A, 123, 8527-8535(2019)

Condensed Matter (2.711)

Rajesh Thakur, P. K. Ahluwalia, Ashok Kumar, Munish Sharma, and Raman Sharma , Helical shaped Graphene Nano-Ribbons: Role of Symmetries and Passivation,. Submitted to a peer-reviewed journal.[arxiv link: https://arxiv.org/abs/1907.00567]

Physics of Fluids (2.627)

Kunjal Shah, Ravi Shakya, Sanjay Mittal, "Aerodynamic forces on projectiles used in various sports",Physics of Fluids, 31, 015106 (2019).

Gaurav Chopra, Sanjay Mittal, coefficient and formation length at the onset of vortex shedding,Physics of Fluids,31(1), 013601 (2019).

Samuthira Pandi Jawahar Sivabharathy, Sanjay Mittal, "Wake transitions and laminar separation bubble in the flow past an Eppler 61 airfoil,Physics of Fluids, 31(11), 114102 (2019).

BBA - Proteins and Proteomics (2.541)

Tajalli Ilm Chandel, Nida Zaidia, Masihuz Zamana, Ishrat Jahan, Aiman Masroor, Ibrar Ahmad Siddique, Shahid M. Nayeem, Maroof Alid, Vladimir N. Uversky, Rizwan Hasan Khan, multiparametric analysis of the synergistic impact of anti-Parkinson's drugs on the fibrillation of human serum albumin. BBA - Proteins and Proteomics 1867 (2019), 275-285

Amino Acids(2.5)

S. S. Narang, D. Goyal, B. Goyal, Molecular insights into the inhibitory mechanism of bi-functional bis-tryptoline triazole against β-secretase (BACE1) enzyme. Amino Acids 2019, 51, 1593-1607.

J. App. Phys (2.328)

N. Kumar, D. Chattaraj, I. Kaul, C. Majumdar, and P. Ghosh, First principles investigation of growth of small Pd-Ga bimetallic clusters on MgO(100) surface, J. App. Phys, 125, 185304 (2019).

Atmosphere (2.14)

Saikia, A., Pathak, B., Singh, P., Bhuyan, P.K. and Adhikary, B., 2019. Multi-Model Evaluation of Meteorological Drivers, Air Pollutants and Quantification of Emission Sources over the Upper Brahmaputra Basin. Atmosphere, 10(11), p.703.; doi:10.3390/atmos10110703.

AIP Advances (1.579)

Barnali Bhattacharya, Jyotirmoy Deb, Utpal Sarkar, "Boron-phosphorous doped graphyne: A near-infrared light absorber", AIP Advances, 9, 095031 (2019).

J Supercond Nov Magn (1.13)

S. Singh, & R. Kumar, Superconducting Properties of LaSn3 Under Positive Hydrostatic Pressure, J Supercond Nov Magn 32, 3431-3436 (2019).

Physica C: Superconductivity and its Applications (0.985)

S. Singh, & R. Kumar, Superconductivity in YIn3 Under Positive Pressure, Physica C: Superconductivity and its applications 564, 6-10 (2019).

International Journal of Computer Applications (0 .704)

Nilesh Maltare ,Vithal N Kamat, Parallel Design Patterns on Molecular Dynamics Simulation, International Journal of Computer Applications. Volume 181 - Number 50, 21-24, April 2019.

AIP Conference Proceedings (0.40)

Ankur Taya, Priti Rani and Manish K. Kashyap, Structural, Electronic and Optical studies of Pb-Free Halide Double Perovskite Cs2BiAgBr6; an mBJLDA approach, AIP Conference Proceedings 2093, 020028 (2019).

Mohammad Ubaid, BS Pujari and A Aziz, "First principle study of In/Ga-doped phosphorene", AIP Conference Proceedings, 2115 (2019) 030392.

Ankur Taya, Renu Singla, Priti Rani, Jyoti Thakur, and Manish K. Kashyap, First principles study of structural, electronic and optical properties of Cs-doped HC(NH2)2PbI3 for photovoltaic applications, AIP Conference Proceedings 2115, 030610 (2019).

Mohammad Ubaid, BS Pujari and A Aziz, "Adsorption of Na atom on mono-layer gallenene", AIP Conference Proceedings, 2142 (2019) 110021.

Materials Today: Proceedings (0.28)

Nishitha P. Mathew, N.Rajeev Kumar and R Radhakrishnan, Lead free Halide Double Perovskites (Cs2AuBiX6: X= Cl, Br)- Potential Light Harvester in Solar Cells, Materials Today: Proceedings, 2020, ISSN 2214-7853,https://doi.org/10.1016/j.matpr.2019.12.022.

J. Ind. Chem. Soc (0.158)

N. Joshi and P. Ghosh, Does semi hydrogenated graphene on lattice matched transition metal substrates has a uniform hydrogen adsorption pattern?, J. Ind. Chem. Soc., 96, 993 (2019) (Special Issue on Theoretical and Computational Chemistry)

Submitted

K. C. Bhamu, Enamul Haque, C.S. Praveen, Nandha Kumar, G. Yumnam, M. Anwar Hossain, Gautam Sharma, Improving the Optical and Thermoelectric Properties of Cs2InAgCl6 with Substitutional Doping: A DFT Insight; arXiv:2001.07337 (2020) Submitted

: Shape dependent Stability and Electronic dispersion of bilayer GrapheneSpirals, Authors: Rajesh Thakur, P. K. Ahluwalia, Ashok Kumar, and Raman Sharma. Submitted

An improved density based compressible flow solver in OpenFOAM for unsteady flow calculations. Submitted to and Mathematics with applicationsDec 29, 2019

Manuscript by S. S. Deshpande, D. B. Potekar, M. D. Deshpande, P. B. Shelke, on study of interaction of Fe13O8@Zn48O48 cluster with dopamine: Magnetic and optical propertiessubmitted to J. Mol. Graph. Mod

Dr. Ashok De, An improved density based compressible flow solver in OpenFOAM for unsteady flow calculations. Submitted to and Mathematics with applicationsDec 29, 2019

Conference/Proceedings:

Dr. Anver Aziz presented (POSTER) a paper entitled of Na atom on Mono-Layer Gallenenein International Conference on Advances in Basic Sciences (ICABS-19) February 7-9, 2019, G.D.C.Memorial College, Bahal (Bhiwani), Haryana, India

Gaurav Chopra, Sanjay Mittal presented work on, formation length near the onset of vortex shedding in flow past a circular cylinder, Asian congress of Fluid Mechanics (2019), JNCASR Bengaluru, India.

Tulsi Ram Sahu, Mohd Furquan, Sanjay Mittal presented work on, study of flow-induced vibration of a circular cylinder with flexible splitter, Asian congress of Fluid Mechanics (2019), JNCASR Bengaluru, India.

Tulsi Ram Sahu, Gaurav Chopra, Sanjay Mittal presented work on, -induced vibration of a circular cylinder at high Reynolds number, Symposium on Fluid-Structure-Sound Interactions

and Control (2019), Chania, Crete Island, Greece.

Dr. Sharanya Sur participated in Conference on Plasma Simula8ons, 23rd - 24th Jan. 2020, Institute for Plasma Research, Gandhinagar

Sandhya Wakhare presented poster in ETMN-2019, International conference held at the Electronics Department, SPPU, Pune in Dec. 2019.

Swapnil Deshpande attended workshop on silico quantum modelling studiesat IUAC, New Delhi from 25th Nov. to 29th Nov. 2019.

Deepali Potekar participated and presented poster in International Conference on Advanced Nanomaterials Nanotechnology. (ICANN- 2019) at S. D. Arts, V. S. A. Commerce M. H. M. Science College, Palghar from 26th to 28th November.

Deepali Potekar participated and presented poster at Dept. of Physics, Sandip University, Nashik from 11th to 12th October 2019.

Sandhya Wakhare presented poster in International conference, on structural, electronic and optical properties of functionalized GaN using DFTin Nanotsav, at Sandip University, Nashik in Oct. 2019.

Sandhya Wakhare presented poster at the RAMAN conference held at SPPU, Pune in Feb. 2019.

Ashima Rawat has presented work in School on Electronic Excitations in Novel Materials Using the Yambo Codeheld in ICTP, Trieste, Italy between 27th and 31st January, 2020

Ashima Rawat participated and presented poster Poster Award (two times) at two ACS sponsored Conferences, ICAN-2019 ICANN-2019 held at IIITM, Gwalior and IIT, Guwahati between 27-29 January, 2019 and 18-21 December, 2019 respectively

Presented (POSTER) a paper entitled and Thermal Properties of In/Ga Doped Phosphorene: A DFT STUDY in an International Conference on Advanced Materials Centre for Nanoscience and Nanotechnology (ICAM-19) March 6-7, Jamia Millia Islamia (Central University), New Delhi.

Dr. K.C. Bhamu presented Poster and got Best Presentation Award in -2019, Govt Science College Sikar (Raj.) During 12-13Feb, 2019.

Dr. Sunita Patel presented work on "Mechanistic insights into mutation induced conformational transition from disordered-to-ordered state in Hahellin, a -crystallin" in the International

conference on Multiscale Simulation & Mathematical Modelling of Complex Biological System held in Jawaharlal Nehru University from Jan 30 to Feb 01, 2019.

Dr. Sunita Patel presented work on induced conformational transition from disordered-to-ordered state in a -crystallin, Hahellinin an one-day symposium on in Biological Systemheld at Tata Institute of Fundamental Research Mumbai on April 27, 2019

Dr. R Radhakrishnan presented work on, Recent advances in Perovskite Solar Cells, Young Investigator Meet On Quantum Condensed Matter Theory, S. N. Bose National Centre for Basic Sciences, Kolkata, 11/12/2019 - 13/12/2019

Dr. R Radhakrishnan presented work on, Effect of Rubidium Doping on the Structural and Opto-electronic Properties of the Halide Double Perovskites Cs(Rb x Cs 1-x)AgBiBr 6 for High Performance Perovskite Solar Cells, International Conference on Photochemistry and Sustainable Energy (ICPSE 2019), St. Michaels College, Cherthala, Kerala, India, 16/10/2019 - 19/10/2019

Dr. R Radhakrishnan presented work on , Tuning the optical properties of Rubidium Doped Cs2InAgBr6 for Solar Cell Applications, International Conference on Photochemistry and Sustainable Energy (ICPSE 2019) St. Michaels College, Cherthala, Kerala, India, 16/10/2019 - 19/10/2019

Dr. R Radhakrishnan presented work on , Direct Bandgap Double Perovskites Cs 2 AgInX 6 (X= Cl, Br) as a Light Absorber in Solar Cells, International Conference on Photochemistry and Sustainable Energy (ICPSE 2019), St. Michaels College, Cherthala, Kerala, India, 16/10/2019 - 19/10/2019

Dr. R Radhakrishnan presented work on , Lead free Halide Double Perovskites (Cs2AuBiX6 : X= Cl, Br)- Potential Light Harvester in Solar Cells, International Conference on Recent Advances in Materials and Manufacturing (ICRAMM 2019), KLE Dr. M S Sheshgiri College of Engineering Technology, Belagavi, Karnataka, India, 12/09/2019 - 14/09/2019

Dr. Ashok De presented Self-induced oscillations of the shock structures in a hypersonic flow over double wedge. Submitted to conference, XXV ICTAM, 23-28 August, 2020, Milan, Italy.

Gupal Singh Khosa Panjab University presented work in International Conference on Condense Matter Physics 2019 at Bikaner and DAE SSPS 2019 at Jodhpur.

Dr. Deepti Goyal's work presented at 25th CRSI National Symposium in Chemistry from 19-21 July, 2019 at Indian Institute of Technology, Kanpur, India

Dr. Deepti Goyal's work presented at Application of Biotechnology in Industry and Society-ABIS-2019 from 14-16 November, 2019 organized by Department of Biotechnology, Dr B R Ambedkar NIT Jalandhar, Punjab, India.

Dr. Deepti Goyalwork presented at 88th Annual Meeting of the Society of Biological Chemists, India (SBCI-2019) and Conference on Advances at the Interface of Biology & Chemistry 2019 from 1-3 November, 2019 at Bhabha Atomic Research Centre, Mumbai, India.

Dr. Gaganpreet presented, Toxic gas adsorption on doped phosphorene: A density functional approach, at IEMPHYS 2019 Kolkata November 2019.

Dr. Gaganpreet presented Poster, Toxic gas adsorption on doped phosphorene: A density functional approach, Graphene 2019, Rome Italy

Dr. Manish Kumar attended and presented a paper entitled , structural, vibrational and magnetic properties of interstitially doped L10-FeNi:N Alloyin 26th WIEN2k Workshop on DFT based simulations of solids with the WIEN2k code at TU, Wien, Vienna, Austria during 13-17 August, 2019.

Dr. Manish Kumar attended and presented a paper entitled of Cs doping on optical absorption of APbI3 (A =-CH3NH3, -CH(NH2)2) hybrid lead iodide perovskitesin third International conference on advanced materials (ICAM 2019) at Mahatma Gandhi University, Kottayam, Kerala during 09-11 August, 2019.

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6

Visits

Total number of visitors during Year-2019 : 2100

6.1 Visits by Dignitaries

- Shri. Ajay Prakash Sawhney, Secretary, MeitY.
- Shri. Jaideep Kumar Mishra, Joint Secretary, MeitY.
- Shri. Sudhir Garg, Joint Secretary, Ministry of Micro, Small & Medium Enterprises.
- Shri. Rinzing Chewang Bhutia, Additional Secretary, Govt. of Sikkim.
- Shri. G.C Khanal, Additional Director, Land Revenue and Disaster Management, Govt. of Sikkim.
- Mr. Vinay Thakur, Chief Operating Officer, Director, (National e-Governance Division) NeGD, MeitY.
- Shri. N. Ravi Shanker, Chancellor DIT University, Dehradun.
- Shri. N.K Mathur, Member (Design & Research), Central Water Commision.
- Col. Ved Pal Yadav.
- Col. A.R Ramakrishnan, Chief Instructor (Nuc) FCBRNP, College Of Military Engineering, Pune.
- Shri. T.P Singh, Director, Bhaskaracharya Institute For Space Applications and Geo-Informatics.
- Shri. S.K Saxena DIG, National Crime Records Bureau (NCRB), Deputy Director.
- Shri. Amitabh Banerjee, Director (Finance), Konkan Railway Corporation Ltd., Mumbai.
- Ms. K.B Vandana, IPS Deputy Inspector General, National Investigation Agency (NIA).
- Sachin Kumar, Scientist , SASE RDC, DRDO Chandigarh.
- Prof. Venkatesh Raghavan, Professor of Geoinformatics, Osaka City University, Japan.
- Dr. K.S Ranjan, Associate Professor, IIIT Hyderbad.
- Mr. Pranab K Rakshit, Chief Manager (R & D), Bharat Petroleum Corporation Ltd.

- R.C Sharma, National Security Council Secretariat.
- Prof. (Dr.) Vijay Gaikwad, Head and Associate Professor, VIT Pune.
- Prof. Vishwajit Balovala, Uka Tarsadia University, Surat, Gujarat.
- Mr. Suhas Punekar, Managing Director, Punekar Educational Initiatives.

6.2 Visits by Academic Institutions

Table 6.1: Summary of Industrial Visits

Institution	No. of visitors
2019	
Amity University Chhattisgarh, Raipur	60
Mahavir Swami College of Engg and Tech	45
MSS 's College of Engg & Tech (Polytechnic Wing), Jalna	35
Shri Vaishnav Vidyapeeth Vishwavidyalaya, Indore	40
Sigma Engineering College, Matar	51
Chhotubhai Gopalbhai Patel Institute of Technology (CGPIT), Bardoli	90
Dr. Jivraj Mehta Institute of Technology, Ahmadabad	40
St. Jhone College of Management, Palghar.	55
Viva Institute of Technology,Virar	30
Sal College of Engineering	86
Anjuman-i-Islam's Akbar Peerbhoy College,Mumbai	100
Mahindra Ecole Centrale, Hyderabad	60
AMTC Trainees, IMD, Pune	12
Pillai College Of Engineering (CSI-PCE), Mumbai	80
Amrutvahini College of Engineering, Sangamner	50
D Y Patil Polytechnic College, Pune	100
Hansba College of Engineering, Gujarat	45
Pune Institute of Computer Technology, Pune	132
Zeal College of Engineering & Research, Narhe, Pune	60
Army Public School Kirkee Pune	120
INS Hamla,Indian Navy	13
JSPM Group of Institutes, Rajarshi Shahu College of Engineering, Pune	30
AISSMSIOIT	30
JMFs Vande Mataram Degree College Dombivli Thane	45
"G.H.Raisoni College of Engineering and Management, Wagholi,Pune"	40
Marathwada Mitramandals College of Engineering, Pune	50
DY Patil College of Engineering,Ambi	80
Pimpri Chinchwad Polytechnic, Akurdi	116
Symbiosis Institute of Geoinformatics	30
Bhagwaan Arihant Institute of technology (BAIT), Surat	45
Trinity Polytechnic, Pune.	40
Collge of Military Engineering	70
NDA, Khadakwasla	30

Continued on next page

Table 6.1 – *Continued from previous page*

Institution	**No. of visitors**
Shri Vaishnav Institute of Technology and Science, Indore MP	50
Vishwakarma Institute of Technology (VIT), Pune	45
MSG SGKM Universal College , Mumbai	50
Gurukul Polytechnic , Nandgaon (Nashik)	45
Total	2100

Appendices

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Appendix A

Financials

Finance section would be covering the over- all expenditures towards running the operations of clusters at NPSF, purchase of spare parts for the NPSF Resources, Commercial Invoices raised for PARAM Yuva II services and the CPU Time Invoices raised regarding the utilization of compute resources of PARAM Yuva II cluster.

Operational expenditure would include the AMCs of Power-Cooling Infra i.e. PAC (Precision Air Conditioners), UPS (Uninterrupted Power Supply), DG (Diesel Generators), Synchronization panel Breaker switch and the charges towards the consumption of electricity and diesel.

Purchase of Spare parts for NPSF includes network cards-cables, power supply units, hard disks, etc. that costs up to Rs. 20 lacs.

In total Year2019 total expenditure comes to around Rs.2 crores.

Commercial Invoices being raised for the users paying the charges towards using the PARAM Yuva II compute resources. In 2019, close to Rs. 1 Lac amount of Commercial Invoices has been raised.

Monthly invoices raised regarding the utilization of compute resources of PARAM Yuva II cluster by user's jobs. Theses invoice being sent to individual Chief Investigator of the Projects during Year2019 (i.e. from January to December). The accumulated value of the CPU time consumed for Year 2019 is 3, 41, 69,482.00 CPU Hours. E-Money Equivalent of the consumed CPU Time is around Rs. 11, 08, 23,840.50 (Eleven Crores Eight Lakhs Twenty Three Thousand Eight hundred Forty only).

Table: Financials

Sr. No.	ITEMS Recieved	INR
1	Total Commercial Invoices raised for the use for PARAM Yuva services	99.8k

Table: Financials

Sr. No.	**Expenditure**	**INR**
1	AMC for PAC	7.5 lac
2	AMC for UPS	6 lac
3	AMC DG Set	1.5 lac
4	AMC for Synchronization Panel	30 k
5	AMC for Breaker Switch	85 k
6	Diesel Comsumed	10 lac
7	Electricity Consumed	160 lac
8	Purhase of Spare Parts for NPSF	20 lac
	Total	**2.06 cr**

Note : Figures in INR mentioned above are not to be considered as exact expenditure Manpower / Staffing cost is not shown

Appendix B

Users across Institutions

Below is the list of NPSF users across Institutions

Table B.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	10
Chandigarh	Panjab University , Chandigarh	8
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	Ahmedabad University,Ahmedabad	2
	Central University of Gujarat (CUG), Gandhinagar	3
	Government Engineering College, Modasa	1
	Indian Institute of Technology (IIT), Gandhi Nagar	10
	Sardar Vallabhbhai National Institute of Technology (SVNIT) , Surat	14
	St. Xaviers College, Ahmedabad	1
Haryana	Central University of Haryana (CUH), Jant-Pali	3
	Kurukshetra University, Kurukshetra	4

Continued on next page

Table B.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	4
Karnataka	Indian Institute of Astrophysics, Bengaluru	12
	Indian Institute of Science (IISC), Bengaluru	7
	LGC Promochem India Pvt Ltd, Bengaluru	1
	Maharanis Science College for Women, Bengaluru	1
	Manipal University, Bengaluru	2
	University of Mysore, Mysuru	2
Kerala	Indian Institute of Science Education and Research (IISER), Thiruvananthapuram	3
	Indian Institute of Space Science and Technology (IIST), Thiruvananthapuram	2
	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 Commerce0College, Jalgaon	1
	College of Engineering (COEP), Pune	8
	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	62
	Indian Institute of Technology (IIT), Bombay	260
	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	43
	Shivaji University, Kolhapur	2
	Swami Ramanand Teerth Marathwada University (SRTMUN), Nanded	2
	Symbiosis Institute of Technology (SIT), Pune	1
	Tetrahydrix Engg. Pvt. Ltd. (TEPL), Pune	1

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Table B.1 – *Continued from previous page*

State	Academic Institutions	No. of Users
	Visvesvaraya National Institute of Technology (VNIT), Nagpur	10
	Whistling Woods International Institute (WWII), Mumbai	2
Mizoram	Pachhunga University College , Aizawl	1
Odisha	Indian Institute of Technology (IIT), Bhubaneswar	6
	Indian Institute of Science Education and Research (IISER),Berhampur	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	2
	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	14
	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	35
	International Institute of Information Technology (IIIT), Hyderabad	4
	Osmania University, Hyderabad	3
	Professor Jayashankar Telangana State Agricultural University0(PJTSAU), Hyderabad	1

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Table B.1 – *Continued from previous page*

State	Academic Institutions	No. of Users
	University of Hyderabad, Hyderabad	1
Uttar Pradesh	Aligarh Muslim University (AMU), Aligarh	7
	Amity University, Noida	2
	Banaras Hindu University, Varanasi.	3
	GLA University, Mathura	1
	Indian Institute of Technology (IIT), Kanpur	30
Uttarakhand	Indian Institute of Technology (IIT), Roorkee	5
West Bengal	Indian Institute of Science Education and Research (IISER), Kolkata	2
	Indian Institute of Technology (IIT), Kharagpur	13
	Total	**774**

Table B.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	10
	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)	157
	CSIR-National Chemical Laboratory (CSIR-NCL), Pune	8
	E-teacher	2
	Inter-University Centre for Astronomy and Astrophysics (IUCAA), Pune	7

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Table B.2 – *Continued from previous page*

State	Research Institutions	No. of Users
	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
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	**419**

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Appendix C

Projects Enrolled during Year 2019

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 C.1: Projects using NPSF compute time

Institution	Project	Research Field	Chief Investigator	No. of users
Aligarh Muslim University (AMU), Aligarh	MD Simulations of Biomolecules	Uncategorized	Dr. Md. Shahid Nayeem	2
Banaras Hindu University, Varanasi	Probing Electronic Structure of Metalloporphyrins in Biological and Supramolecular Environments.	Uncategorized	Dr. Tulika Gupta	3
Biological and Life Sciences, Ahmedabad University	Drug Design and Molecular Simulation Studies of Beta and Gamma Secretase and Beta Amyloid Proteins and Other Proteins Involved in Neurodegeneration Diseases	Uncategorized	Dr. Vivek Tanavde	2
College of Engineering (COEP), Pune.	classification in Images and Videos using deep learning architecture	Uncategorized	Dr. Sunil B. Mane	2
CSIR-National Chemical Laboratory (CSIR-NCL), Pune.	Investigations of thermoelectric performance of mixed metal organo halides: CH3NH3AB3	Material Sciences	Dr. K C Bhamu	1
Government Engineering College, Modasa (gecmodasa)	Adaptive Parallel Design Pattern for Multicore	Computational Sciences	Mr. Nilesh Maltare	1
H.P.T Arts and R.Y.K. Science College, Nasik.	Theoretical investigation of structural, electronic, magnetic and optical properties of undoped and doped iron oxide nanostructures.	Others	Dr. Dattatraya Laxman Lalsare	1
	Theoretical study of Structural, Electronic and Magnetic Properties of Nanomaterials	Material Sciences	Dr. M.D. Deshpande	2

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Table C.1 – *Continued from previous page*

Institution	Project	Research Field	Chief Investigator	No. of users
	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	2
Indian Institute of Astrophysics (IIAP), Bengaluru	Numerical simulations of Hydromagnetic turbulence from galaxies to Sun	Astronomy and Astrophysics	Dr. Sharanya Sur	2
Indian Institute of Science Education and Research (IISER), Pune.	Study of coupled quantum hall systems	Uncategorized	Dr. Sreejith Ganesh Jaya	2
Indian Institute of Science Education and Research (IISER),Berhampur	Computational Study for drug delivery using Metal-Organic Frameworks as a carrier	Uncategorized	Dr. Malay Kumar Rana	2
	Exploring the protein stability and flexibility by comparative molecular dynamics simulation of homologous Hyperthermophilic	Uncategorized	Dr. Malay Kumar Rana	2
	Structure based drug designing and molecular dynamics studies of Plasmepsins of Plasmodium Falciparum for malaria	Uncategorized	Dr. Malay Kumar Rana	3

Continued on next page

Table C.1 – *Continued from previous page*

Institution	Project	Research Field	Chief Investigator	No. of users
Indian Institute of Science Education and Research(IISER), Mohali	Two dimensional layered materials for toxic gas sensing applications using density functional theory based approaches	Uncategorized	Dr. Gaganpreet	1
Indian Institute of Space Science and Technology (IIST), Thiruvananthapuram	"Force field development for heteroatoms for optimization of carrier Mobility in OLED devices "	Uncategorized	Dr. Nirmala Rachel James	2
Indian Institute of Technology (IIT), Bhubaneswar.	Multiscale modeling of layered 2D materials for energy and electronics applications	Uncategorized	Dr. Hemant Kumar	1
Indian Institute of Technology (IIT), Hyderabad.	First principles investigation of magnetic materials and superconductors	Uncategorized	Prof. Venkata Krishnan Kanchana	2
	First principles investigation of topological materials	Uncategorized	Prof. Venkata Krishnan Kanchana	2
	First principles investigation of thermoelectric materials	Uncategorized	Prof. Venkata Krishnan Kanchana	2
	Tuning the Spin Polarisation of Heusler Intermetailics towards Spintronic Applications	Uncategorized	Prof. Venkata Krishnan Kanchana	2
Indian Institute of Technology (IIT), Jodhpur.	Theoretical / DFT studies (phonon calculations, electrical and optical properties) on semiconductors.	Uncategorized	Dr. Ambesh Dixit	3
Indian Institute of Technology (IIT), Patna.	Quantum Transport phenomena in Nano scale devices	Uncategorized	Dr. Jawar Singh	2

Continued on next page

Table C.1 – *Continued from previous page*

Institution	Project	Research Field	Chief Investigator	No. of users
Indian Institute of Technology (Indian school of Mines) (IITISM) , Dhanbad	Three Dimensional modelling of Magnetotelluric Data over Dalma and Dhanjori Volcanics	Uncategorized	Prof. Shalivahan	3
Indian Institute of Technology, Bombay (IITB)	Materials modelling for potential thermoelectric, solar and topological materials.	Uncategorized	Prof. Aftab Alam	2
	Face approach to molecular spintronics materials.	Uncategorized	Prof. Gopalan Rajaraman	2
	Density Functional theory calculations	Uncategorized	Prof. Subhananda Chakrabarti	2
	Direct Simulation Monte Carlo for rarefied gas flows in complex microchannel (2D and 3D)	Uncategorized	Prof. Amit Agrawal	2
	Functional annotation of proteins based on binding site characteristics	Uncategorized	Prof. P.V. Balaji	2
	Molecular dynamics simulations of aggregation of anti-microbial peptides into amyloidogenic assemblies	Uncategorized	Prof. Ajay Singh Panwar	2
Indian Institute of Technology, Kanpur (IITK)	Hypersonic Flow and Heat Transfer	Uncategorized	Dr. Ashoke De	5
Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR), banglore	Atomistic MD simulations of fumarate hydratase enzyme	Uncategorized	Prof. Balasubramanian Sundaram	1

Continued on next page

Table C.1 – *Continued from previous page*

Institution	Project	Research Field	Chief Investigator	No. of users
Kurukshetra University, Kurukshtra	Simulations of rare earth free magnetic inorganic halide perovskites for photovoltaic applications, Academic	Uncategorized	Dr. Manish Kumar Kashyap	4
Maharani's Science College for Women, Bengaluru	First Principles calculations of 2D Materials such as Phosphorene and TMDS	Uncategorized	Dr. G. Sriprakash	1
Osmania University, Hyderabad.	Modeling & Simulations of Materials	Uncategorized	Dr. Moumita Saharay	2
Panjab University , Chandigarh	Electronic and thermal properties of thermoelectric materials.	Uncategorized	Dr. Shuchi Gupta	2
S. N. Bose National Center for Basic Sciences, Kolkata	Molecular mechanism of signal transduction ,protein-protein interaction and allosteric regulation	Uncategorized	Dr. Suman Chakrabarty	1
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	6
	Development of Novel Cluster Assembled Materials from Potential Cluster Motifs: A New Insight under Density Functional Investigation	Material Sciences	Dr. Debesh R. Roy	6
Savitribai Phule Pune University, Pune.	Exploring Density Functional Probing noncovalent interactions from density functional theory	Computational Sciences	Prof. Shridhar P Gejji	5
	Electornic Properties of double perovskites	Uncategorized	Prof. S.V.Ghaisas	2

Continued on next page

Table C.1 – *Continued from previous page*

Institution	Project	Research Field	Chief Investigator	No. of users
	Computational studies of B1 adrenergic receptor	Uncategorized	Dr. Manali Joshi	2
	Simulation of bremsstrahlung spectrum generated by medical linac and neutron spectrum generated by high energy proton beam using Monte Carlo based Geant4 code	Uncategorized	Prof. Sanjay D. Dhole	2
Shivaji University, Kolhapur.	A Study of Anisotropic Thermal Conductivity of Graphene by Molecular Dynamics Simulation.	Uncategorized	Dr. R. S. Vhatkar	2
Sri Guru Granth Sahib World University, Punjab	Design, Synthesis and Evaluation of Modified Short Peptides as Inhibitors of Amyloid-B (AB) Peptide Aggregation	Chemical Sciences	Dr. Deepti Goyal	5
St. Xaviers College, Ahmedabad	Quantum transport in elemental doped boron nitride monolayer	Material Sciences	Dr. Sanjeev Kumar Gupta	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 Rajasthan,Jaipur	Observations of Gold Based Nanocatalysis at nanoscale	Computational Sciences	Dr. Devendra Kumar Mahawar	1
Visvesvaraya National Institute of Technology (VNIT), Nagpur	First priniciple study of some topological materials	Uncategorized	Dr. Poorva Singh	2

*Uncategorized : Projects for which no information on research field was provided by their respective Chief Investigators

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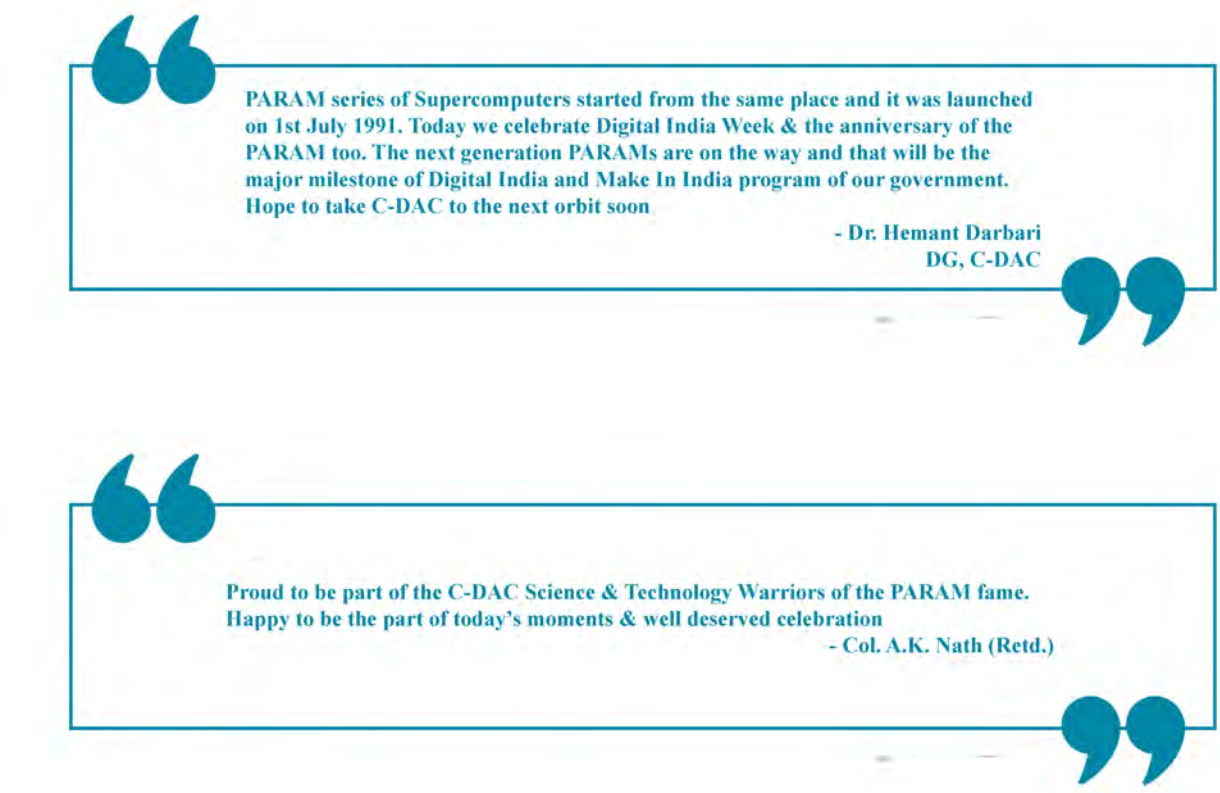
Appendix D

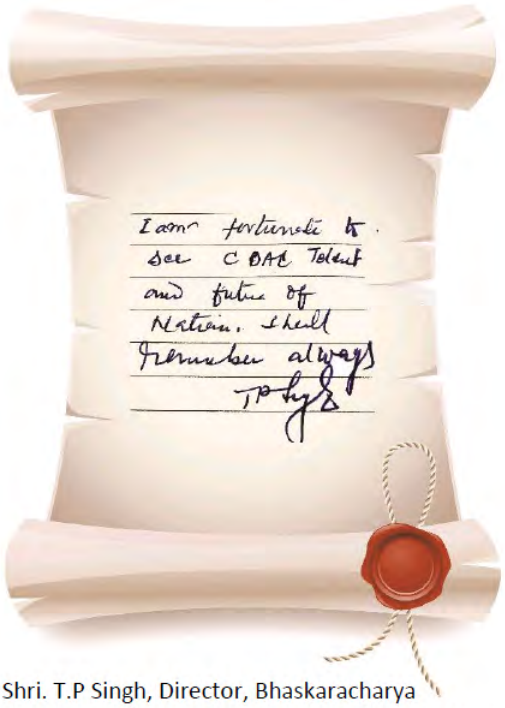
Quotes by Dignitaries & Visitors



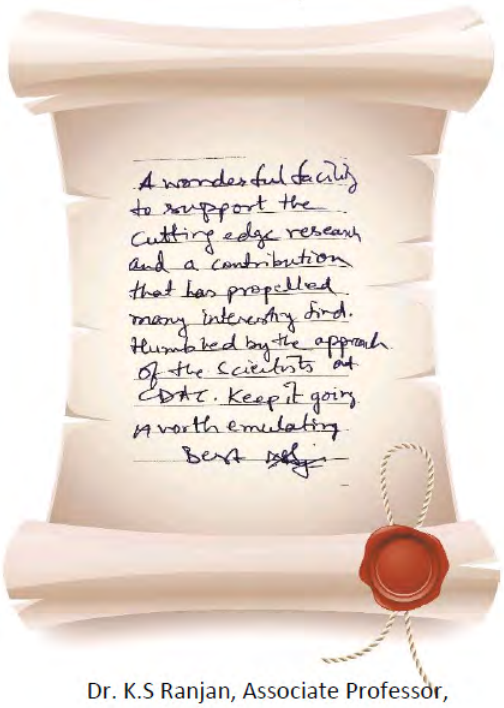
Messages from DG, C-DAC and ED, C-DAC Pune on NPSF Foundation Day (25^{th} July, 2019).

Prof. Venkatesh Raghavan, Professor of Geoinformatics, Osaka City University, Japan

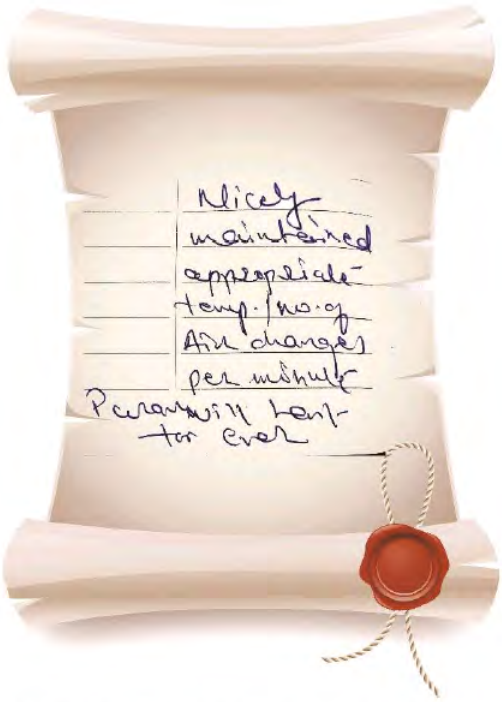
Vinay Thakur, NEGD, MeitY Chief Operating Officer, Director, (National e-Governance Division) NeGD, MeitY



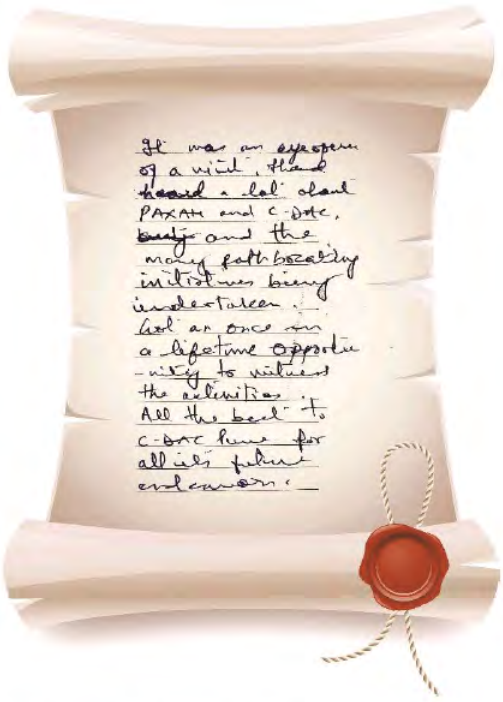
Shri. T.P Singh, Director, Bhaskaracharya Institute For Space Applications and Geo Informatics



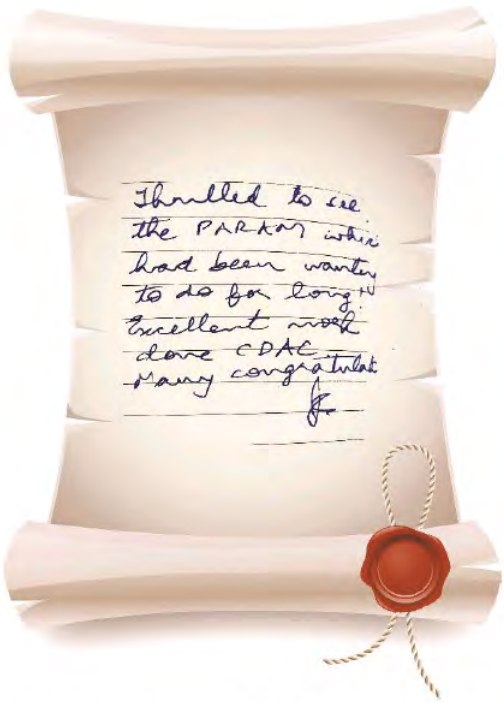
Dr. K.S Ranjan, Associate Professor, IIIT Hyderabad



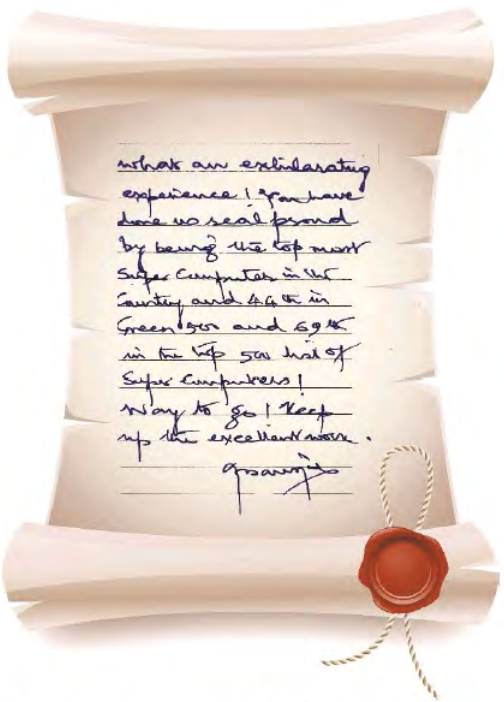
Mr. Suhas Punekar, Managing Director, Punekar Educational Initiatives



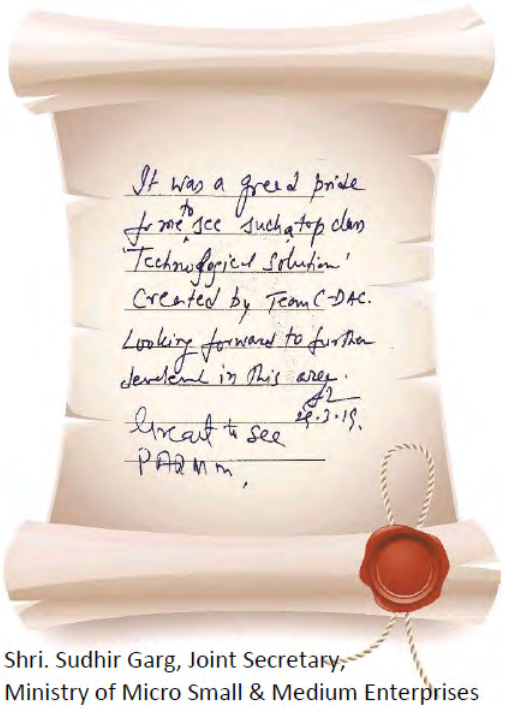
Shri. Rinzing Chewang Bhutia, Additional Secretary, Govt. of Sikkim.
Shri. G.C Khanal, Additional Director, Land Revenue and Disaster Management, Govt. of Sikkim.



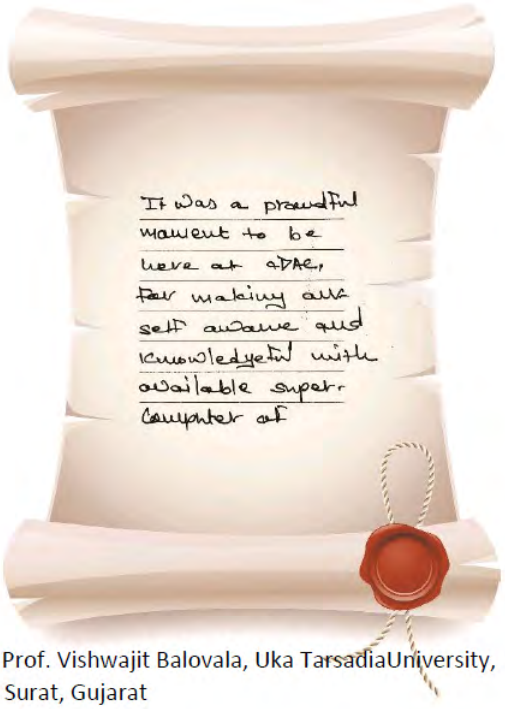
Shri. Jaideep Kumar Mishra, Joint Secretary, MeitY



Shri. Amitabh Banerjee, Director (Finance), Konkan Railway Corporation Ltd., Mumbai



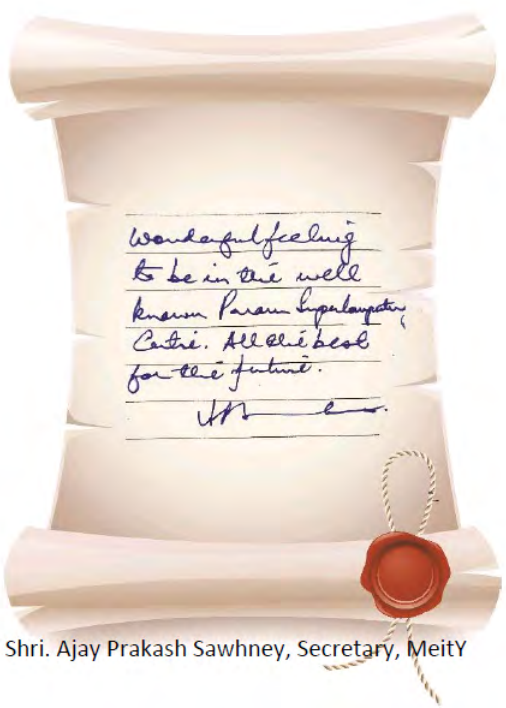
Shri. Sudhir Garg, Joint Secretary,
Ministry of Micro Small & Medium Enterprises



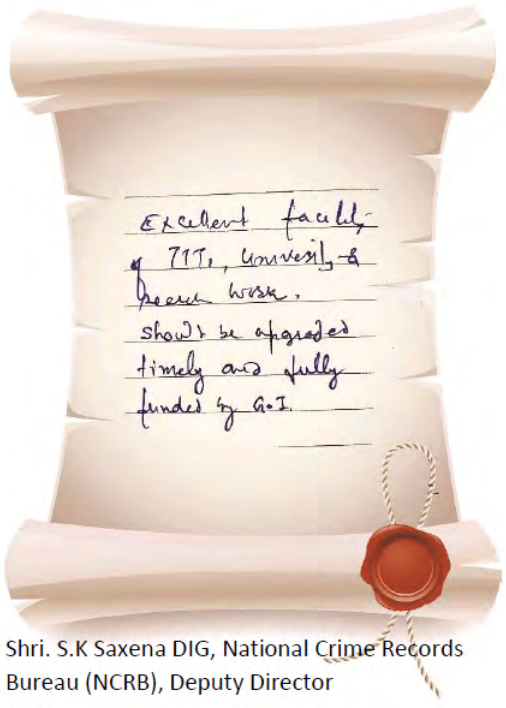
Prof. Vishwajit Balovala, Uka TarsadiaUniversity,
Surat, Gujarat

Shri. N. Ravi Shanker, Chancellor DIT University,
Dehradun

Sachin Kumar, Scientist 'E', SASE RDC,
DRDO, Chandigarh



Shri. Ajay Prakash Sawhney, Secretary, MeitY



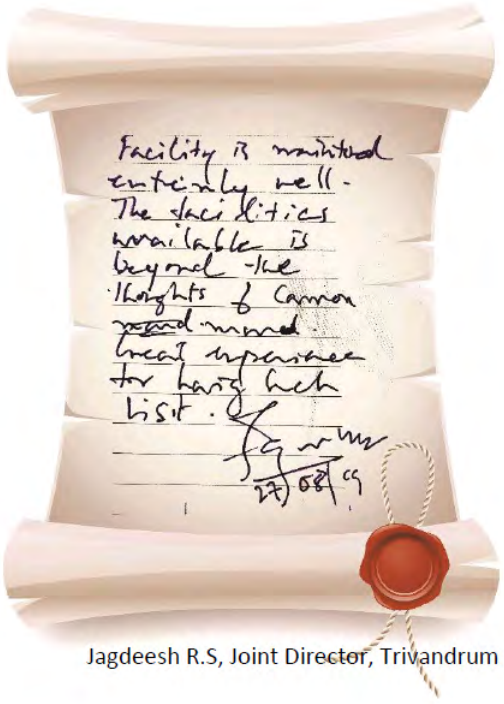
Shri. S.K Saxena DIG, National Crime Records Bureau (NCRB), Deputy Director

Mr. Pranab K Rakshit, Chief Manager (R & D), Bharat Petroleum Corporation Ltd

Col. Ved Pal Yadav

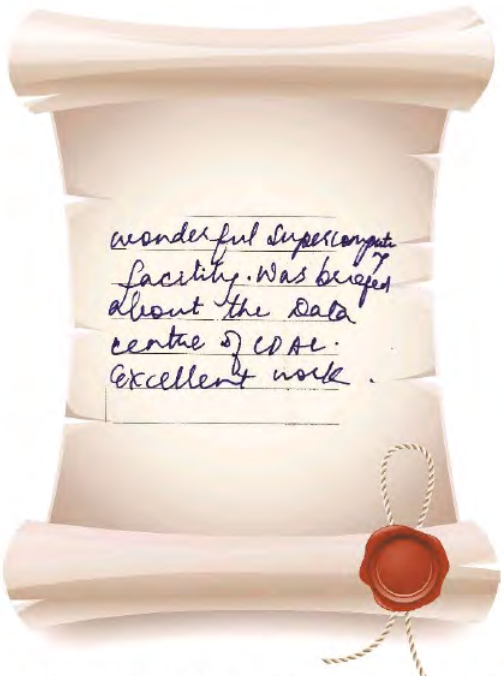
Mr. R.C. Sharma

Col. A.R Ramakrishnan, Chief Instructor (Nuc) FCBRNP, College Of Military Engineering, Pune



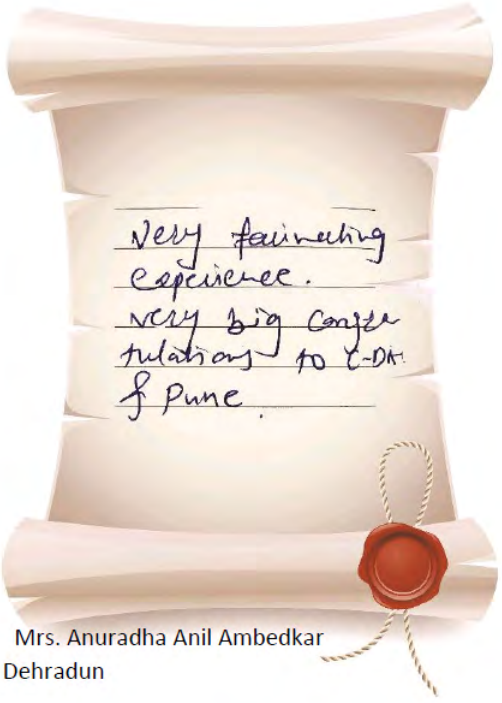
Jagdeesh R.S, Joint Director, Trivandrum

Prof. (Dr.) Vijay Gaikwad, Head and Associate Professor, VIT Pune



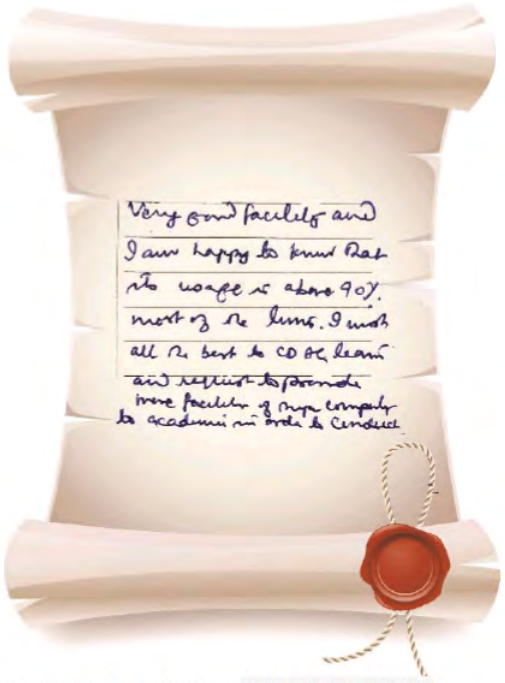
Ms. K.B Vandana, IPS Deputy Inspector General,
National Investigation Agency (NIA)

Sanjit Chaudhary



Mrs. Anuradha Anil Ambedkar
Dehradun

Mr. Pankaj Mishra, Survey of India,



Dr. Santosh K. Pandey, **Scientist C, MeitY**

Appendix E

Picture Gallery

Visit to NPSF by Ms. K. B. Vandana, DIG, NIA, New Delhi.

Visit to NPSF by School Students, Pune.

Visit to NPSF by NIA Officers, New Delhi.

"Seeking inputs from HPC Applications towards the planning of NextGen HPC system" Workshop

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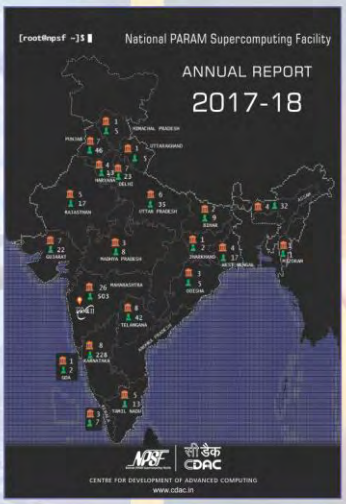
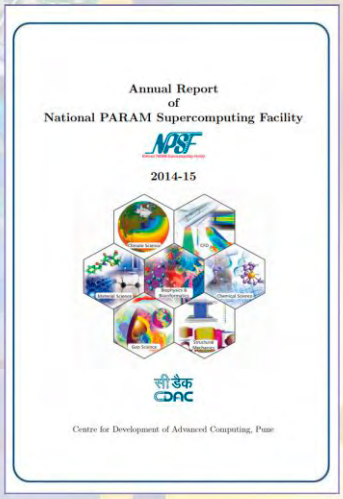
2018



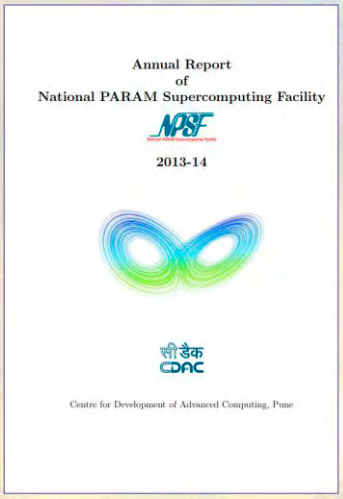
2017-18

2016-17

2015-16



2014-15



2013-14

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