## Department of Computational Sciences Minutes of meeting of Academic and Administrative Committee of Department of Computational Sciences

The meeting of Academic and Administrative Committee of Department of Computational Sciences was held on 09-01-2020 at 2:30 PM. in the Computational Sciences lab cum classroom of Academic block. The following members were present:

1. Dr. Kousik Giri

(Convener)

2. Dr. Sudip Chakraborty

(Chairperson)

The following points were discussed and resolution made:

Item No. 1: The AAC resolves that the following workstations are allotted for the following faculty members to cater their computer intensive research work. The details of allotted workstations have been tabulated in Annexure 1.

Item No. 2: The Department of Computational Sciences (DCS) has established Graphics Processing Unit (GPU) based High Performance Computing (HPC) Laboratory to handle the departmental computer intensive research projects for M.Sc. and Ph.D. students.

The AAC notes that due to heavy demand of computer time for intra Item No. 3: departmental computer based research, presently, DCS - HPC lab has opened six high end desktop and workstations for other departmental computer intensive research, based on their need on first cum first serve basis.

The AAC resolves the format of HPC - Lab access request form Item No. 4: (Annexure 2).

The Department of Computational Sciences is going to organize a twoday workshop on Molecular Modeling and Design, Bioinformatics from 24/02/2020 to 25/02/2020.

The AAC resolves that the department shall process the syllabii through Item No. 6: the BOS in the  $3^{11}$  or  $4^{12}$  week of January 2020.

The AAC notes that the expenditure of INR. 30000/- for imprest amount and INR. 33,300/- for Vch No. 3831(1) from departmental recurring budger till Dissudip Charlaborty 09/01/2020.

Dr. Kousik Giri Kourik Giri 09/01/2020

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## Department of Computational Sciences Minutes of meeting of Academic and Administrative Committee of the Department of Computational Sciences

The meeting of the Academic and Administrative Committee (AAC) of the Department of Computational Sciences was held on 16-10-2020 through online mode.

The following members were present:

1. Dr. Kousik Giri

2. Dr. Sudip Chakraborty

(Chairperson)

3. Dr. Dharmendra Singh

(Convener)

The following points were discussed and resolution made:

**Item 1.** The Department of Computational Sciences (DCS) is taking care of all precautions from COVID 19 and also strictly follow the guidelines, which are issued by the GOI/State/University administration. We are conducting all the classes/meetings/audit by online modes.

**Item 2.** The AAC notes that the DCS has purchased a VASP software license of six (06) users with source codes, among of them the three (03) primary licensees are Dr. Kousik Giri, Dr. Sudip Chakraborty and Dr. Dharmendra Singh.

**Item 3.** The AAC notes that the DCS has completely moved to Gudda campus since 1<sup>st</sup> September, 2020. DCS is still arranging all the stuffs for department and also for laboratory.

**Item 4.** The AAC notes Dr. Dharmendra Singh received University Research Seed Money (RSM) grant for two years since June 2020. He wants to purchase the following items through his project fund.

- a. A work station
- b. A printer
- c. Other office utilities

**Item 5.** The AAC notes that Dr. Sudip Chakraborty requires a laptop for his project management (Project: GP123, CUPB-RSM) and online teaching/ research presentations, the approximate specifications for which 8GB RAM or better, HDD of 1TB or better, i7 processor of 7<sup>th</sup> gen or better. In addition, he is intending to purchase few desktop/workstations, the approximate specifications for which 8GB RAM or better, HDD of 1TB or better, i7 processor of 7<sup>th</sup> gen or better, based on the availability of the CUPB-RSM fund.

**Item 6.** The AAC notes that the DCS is providing a departmental workstation (HP-Z840) to Dr. Dharmendra Singh to initiate his research / online teaching.

**Item 7.** The AAC notes that one of our senior Ph.D. student Mr. Saurav Jindal, who did most of his research work in departmental research lab at CUPB, City Campus. Where, he stored most of his research documents and related data in one departmental iMAC and a workstation HP-Z420. The department is temporarily providing the two systems to Mr. Saurav Jindal for completion of

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his Ph.D. work, and after completion the Ph.D. work he will return the mentioned two systems to the department (DCS).

- **Item 8.** The AAC nominate the name Dr. Dharmendra Singh for the task to collect data about publications and projects of the department and submit it to IQAC on a quarterly basis.
- **Item 9.** The AAC nominate the name Dr. Sudip Chakraborty for the task of placement of students at the department level.
- **Item 10.** Visiting faculty: In view of the notice dated 14/09/2020, the DCS has contacted with two renowned faculty members in the field of Theoretical and Computational Sciences for Visiting Professor position. The names are listed below,
  - 1. Prof. Kalidas Sen (FASc, FNA, INSA Senior Scientist)
  - 2. Prof. Alok Bhattacharyya (FASc, FNASc, FNA, SSB Prize)

Among the above two, Prof. Kalidas Sen has asked few questions related to the position, and the reply email is in Annexure I.

- **Item 11**. The AAC notes the DCS has successfully organized a webinar on 15/10/2020 at 3:00 PM, the title of the webinar was "Career Opportunities and Related Skill Set for High Performance Computing".
- **Item 12.** The AAC notes that due to the reason of the absence of any computer related technical staff (STA) in the Department and the presence of very limited computational facilities, the Department of Computational Sciences is temporarily postponed the uses of departmental computational facility for inter departmental users.
- **Item 13.** The AAC is requesting individual faculty members to start webinar series related to their field of interest.

| Faculty Name<br>Dr. Kousik Giri | Research Interest Theoretical and computational Chemistry                        | Proposed Title for Webinar   |
|---------------------------------|--|--|
| Dr. Sudip<br>Chakraborty        | Molecular Modeling and CPU-GPU Hybrid Computing                                  | <ol> <li>Recent Advances in Molecular<br/>Simulation Methods</li> <li>Bioinformatics and Chemical<br/>Biology Webinar Series</li> </ol>                |
| Dr. Dharmendra<br>Singh         | Mathematical modeling of amorphous material, Amorphous Phase separation dynamics | <ol> <li>Present Scenario in modeling of<br/>Short Range Ordering clusters</li> <li>Fabrications of 2D Materials and<br/>their Applications</li> </ol> |

**Item 14.** The AAC notes that Dr. Kousik Giri, Dr. Sudip Chakraborty and Dr. Dharmendra Singh are temporarily allowed to give a monitor individually from computational lab till then they have own monitor from University Administration/Project Grant/elsewhere.

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Dr. Kousik Giri

Dr. Sudip Chakraborty

Dr. Dharmendra Singh