Curriculum Vitae

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C/O Dr. M L Srivastava
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Career Summary

Research scholar at Indian Institute of Technology (IIT), Jodhpur with overall good academic records at both UG and PG levels. Hold expertise in the field of Molecular Dynamics Simulations of Soft Matters and employing the theoretical concepts of Physical Chemsitry. Core research skills include description of mechanism and energetics of self-aggregation of molecules with biological importance.
Clear communicator of both written and oral. Significantly experienced in handling students of both undergraduate and postgraduate levels. Facilitated learning by developing fundamental concepts and discipline in the pupils. Strong intersocial skills; good articulation with coworkers and officials. Excel in performing under utmost workload and meet competing deadlines.

Subjects of Expertise: All sub-disciplines of Chemistry, Specializations include Inorganic Chemistry, Computational Chemistry.

Research Expertise: Computational Chemistry, Molecular dynamics, All-atom simulations, Coarse-grained simulations, Electronic Structure Calculations, Force-field parameterization, Aggregation, Micelles, Bilayers, Soft-matters, Surfactants, Lipids, Peptides.

Education

Ph.D
2015-current
Department of Chemistry, Indian Institute of Technology, Jodhpur
Thesis: Self-assembly of mixed surfactants and π-conjugated peptide derivatives from multiscale simulations

M.Sc. Chemistry
2013-2015
Department of Chemistry, Jamia Millia Islamia
Thesis: Synthesis, Characterization and Study of Catalytic Activity of Amino Acid Metal Complexes
CGPA: 8.38

B.Sc. (H) Chemistry
2010-2013
Department of Chemistry, Daulatram College, University of Delhi
Percentage: 76.26

Awards and Honors

- Best Poster award at International Conference on advances in Basic Sciences (2019).
- Senior Research Fellowship, awarded by MHRD (2018-present).
- Junior Research Fellowship, awarded by MHRD (2015-2018).
- Eligibility for lecturership, awarded by University Grants Commision (UGC), AIR-22 (2015).
- Graduate Aptitude Test in Engineering (GATE), AIR-431, Percentile-96.34 (2015).

Professional Experience

- **Teaching Assistant**, Department of Chemistry, Indian Institute of Technology, Jodhpur (January 2020-Present)
  Course: Physical Chemistry Laboratory, (M.Sc. level)
- **Teaching Assistant**, Department of Chemistry, Indian Institute of Technology, Jodhpur (January 2020-Present)
  Course: Hands-on Laboratory, (M.Sc. level)
- **Teaching Assistant**, Department of Chemistry, Indian Institute of Technology, Jodhpur (July 2018-December 2018)
  Course: CY211 Laboratory (B.Tech Level)
- **Teaching Assistant**, Department of Chemistry, Indian Institute of Technology, Jodhpur (January 2018-April 2018)
  Course: Chemical Binding Laboratory (M.Sc. Level), Trained M.Sc. with softwares relevant to Computational Chemistry Simulations.

List of Publications

- Molecular dynamics simulations of a stacked π-conjugated soft material: binding energy and preferential geometry for self-assembly, **Arpita Srivastava**, Avinash Garg, Debapratim Das and Ananya Debnath, Bulletin of Materials Science (Invited for Thematic issue on Soft Materials), 2019 (accepted).
- Unusual confinement properties of a water insoluble small peptide hydrogel, Nilotpal Singha, **Arpita Srivastava**, Bapan Pramanik, Sahnawaz Ahmed, Payel Dowari, Sumit Chowdhuri, Basab Kanti Das, Ananya Debnath and Debapratim Das, Chemical Science, 2019, *10*, 5920.
- Cylindrical to Spherical Shape transformations of Micelles using All-Atom and Coarse-Grained Molecular Dynamics Simulations, **Arpita Srivastava** and Ananya Debnath, AIP Conference Proceedings, 2019, *2142*, 130004.
- Solvent Assisted Tuning of Morphology of a Peptide-Perylenediimide Conjugate: Helical Fibers to Nano-Rings and their Differential Semiconductivity, Sahnawaz Ahmed, Bapan Pramanik, K. N. Amba Sankar, Abhinav Srivastava, Nilotpal Singha, Payel Dowari, **Arpita Srivastava**, Kallol Mohanta, Ananya Debnath and Debapratim Das, Scientific Reports, 2017, *9485*, 1.
- Influence of water concentrations on the phase transformation of a model surfactant/co-surfactant/water system, Raju Lunkad, **Arpita Srivastava** and Ananya Debnath, Chemical Physics, (2017) *483-484*, 103.
- Entropy and interdigitation induced asymmetry in mixed surfactant bilayers from all-atom and coarse-grained simulations, **Arpita Srivastava** and Ananya Debnath (manuscript under prepration).

Conferences and Symposia

- Theoretical Chemistry Symposia (TCS), BITS Pilani, February 2019.
- International Conference on Advances in Basic Sciences (ICABS), Bahal, Haryana, February 2019.
- International Conference on Complex and Functional Materials (ICCFM), SNBNCBS, Kolkata, December 2018.
- International Conference on Complex Fluids and Soft Matter, (COMPFLU), IIT Roorkee, December 2018.
- Annual Meeting of the Indian Biophysical Society (IBS), IISER Pune, March 2018.
- Asia Pacific Conference on Theoretical and Computational Chemistry (APCTCC), IIT Mumbai, December 2017.
- Recent Advances in Chemistry (RAC), Jamia Millia Islamia, March 2015.
- Recent Advances in Chemistry (RAC), Jamia Millia Islamia, March 2014.

Skills

Computer Skills: Windows, Linux, MS Office (PowerPoint, Word, Excel), LibreOffice (Writer, Calc, Impress), Shell Script, LaTex.

Softwares: GROMACS, Gaussian, GAMESS (US), NWChem, VOTCA, Grace, VMD, DFTB+, MATLAB, GIMP, Inkscape, Adobe Illustrator, XFig, ATB, PRODRG.

Additional Information

Nationality: Indian

Date of Birth: May 26, 1992

Marital Status: Unmarried

Languages: English, Hindi

References

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