

# Rohit Modee.

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🌐 Rohit Modee

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## Summary

I am a computational chemist and machine learning researcher focusing on atomistic simulations, molecular geometry optimization, and 3D-structure generation. Some of my work includes 3D structures generation using reinforcement learning, benchmarking deep neural network potentials, and developing reinforcement learning methods for molecular geometry optimization. I am passionate about applying my skills to solve real-world problems in drug discovery, materials science, and environmental sustainability.

## Education

- 2018 – . . . . **Ph.D., International Institute of Information Technology (IIIT), Hyderabad, India.**  
CGPA - 9.13/10.  
Thesis title: *Machine learning for molecular geometry optimization and 3D structure generation.*  
Supervisor: Prof. U. Deva Priyakumar
- 2010 – 2015 **M.Tech. (Integrated) in Biotechnology, D.Y. Patil School of Biotechnology and Bioinformatics, Mumbai, India.**  
Percentage 69%.  
Thesis title: *Electron Beam Treatment: Enhancing Fish Shelf Life and Minimizing Bacterial Load.*
- 2008 – 2010 **H.S.C 10+2, S.I.W.S college of science and commerce, Mumbai, India.**  
Percentage 70%.

## Work Experience

- 2015 – 2017 **Junior Research Fellow (JRF), International Institute of Information Technology (IIIT), Hyderabad, India.**  
Principal Investigators (PIs): *Prof. Abhijit Mitra, Dr. Nita Parekh, et. al.*  
As part of the team, I contributed to the development and testing of scripts and algorithms for the Computational Core for Plant Metabolomics (CCPM) web application which serves as a Laboratory Information Management System (LIMS) for processing large volumes of plant metabolomics data.  
WebApp: <http://metabolomics.iiit.ac.in/wiki/about>
- 2015 – 2015 **Dissertation Project, Board of Radiation & Isotope Technology (BRIT-BARC), Navi Mumbai, India.**  
Principal Investigators (PIs): *Dr. K.P. Rawat and Dr. Chanda Arjun.*  
Conducted a research study on the use of 5MeV Electron Beam (EB) treatment for commercial sterilization of lab plastic consumables and depyrogenation of glass vials. Successfully stored basa fish at 3°C using EB treatment, resulting in lower storage costs and power consumption.

## Research Publications

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- 1 **R. Modee**, S. Mehta, S. Laghuvarapu, and U. D. Priyakumar, "MolOpt: Autonomous Molecular Geometry Optimization Using Multiagent Reinforcement Learning", *J. Phys. Chem. B*, 1–27 (2023).
- 2 **R. Modee** and U. D. Priyakumar, "MolOpt2: Understanding and correcting pathologies in developing learned molecular geometry optimizer", 2023, **in press**.
- 3 **R. Modee**, A. Verma, K. Joshi, and U. Deva Priyakumar, "MeGen - generation of gallium metal clusters using reinforcement learning", *Mach. Learn. Sci. Technol.* **4**, 025032 (2023).
- 4 D. B. Korlepara, C. S. Vasavi, S. Jeurkar, P. K. Pal, S. Roy, S. Mehta, S. Sharma, V. Kumar, C. Muvva, B. Sridharan, A. Garg, **R. Modee**, A. P. Bhati, D. Nayar, and U. D. Priyakumar, "PLAS-5k: Dataset of Protein-Ligand Affinities from Molecular Dynamics for Machine Learning Applications", *Sci. Data* **9**, 1–10 (2022).
- 5 **R. Modee**, S. Laghuvarapu, and U. D. Priyakumar, "Benchmark study on deep neural network potentials for small organic molecules", *J. Comput. Chem.* **43**, 308–318 (2022).
- 6 **R. Modee**, S. Agarwal, A. Verma, K. Joshi, and U. D. Priyakumar, "DART: Deep learning enabled topological interaction model for energy prediction of metal clusters and its application in identifying unique low energy isomers", *Phys. Chem. Chem. Phys.* **23**, 21995–22003 (2021).

## Skills

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Computational chemistry software	📖	RDKit, ASE, CHARMM & CHARMM-GUI, NAMD, Gaussian, Packmol, Avogadro.
Computational chemistry methods	📖	Molecular dynamics (MD), Replica Exchange Molecular Dynamics (REMD).
Programming skills	📖	Python, R, PyTorch, L <sup>A</sup> T <sub>E</sub> X, Basic knowledge C/C++, Perl, Bash, UNIX.
Visualization and plotting tools	📖	VMD, GaussView, Gnuplot, Matplotlib (python).
Databases and Web Dev	📖	Basic knowledge of MySQL, SQLite. HTML, CSS, JavaScript, Apache Web Server.
Soft skills.	📖	Academic research, writing research papers, mentoring students, teaching, and consultation. Good communication skills (gave presentations, posters and talks in various conferences).
Languages	📖	English, Hindi and Marathi (can read, write and speak). Telugu and Kannada (can speak).

## Conferences

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### Talk

- 2023 📖 **Machine Learning for Molecular Sciences (ML4Science), 2023**  
International Institute of Information Technology (IIIT), Hyderabad, India.  
Talk on "MeGen: Generation of Gallium Metal Clusters Using Reinforcement Learning."
- 2022 📖 **Molecular Simulation: Focus on Method**  
Tata Institute of Fundamental Research (TIFR), Hyderabad, India.  
Talk on "OptNet: Molecular Geometry Optimization Using Reinforcement Learning."

## Conferences (continued)




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### Poster

- 2022  **Designing Catalysts on Computers (DCC)**  
Indian Association for the Cultivation of Science (IACS), Kolkata, West Bengal.  
Presented poster titled:- "OptNet: Molecular Geometry Optimization Using Reinforcement Learning."
- 2020  **The virtual 3rd RSC-BMCS / RSC-CICAG Artificial Intelligence in Chemistry.**  
Presented poster titled:- "Neural network potentials for representing potential energy surface and their applicability for geometry optimization."
-  **Machine learning how to coarse-grain, CECAM.**  
Co-organised by Dr. Denis Andrienko (Max Planck Institute for Polymer Research) and Dr. Tristan Bereau (University of Amsterdam).
- 2019  **Workshop and Symposium on Advanced Simulation Methods: DFT, MD and Beyond.**  
Indian Institute of Technology (IIT) Delhi, New Delhi, India.  
Presented poster titled:- "Cosolvents Effect on Protein (Un)Folding Equilibrium."
-  **Indian Peptide Society (IPS) 7th Symposium.**  
Birla Institute of Technology and Science (BITS) Pilani, Hyderabad, India.  
Presented poster titled:- "Synergistic Play of Cosolvents in Protein Folding/Unfolding Equilibrium."
-  **Machine Learning For Science (ML4Science).**  
International Institute of Information Technology (IIIT), Hyderabad, India.

## Awards and Achievements




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-  Awarded the prize for best method in a machine learning hackathon focused on property prediction using SMILES at the ML4Science-2023 Meeting.
-  Awarded four year scholarship for Ph.D. by TCS Research Scholar Program (RSP) 2019.
-  Qualified GATE-2015 in biotechnology with 85.54 percentile (All India Rank (AIR) - 1290).

## Miscellaneous Experience

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### Teaching Assistant-ship (IIIT)

-  Data Driven Drug Discovery
-  Advanced Biomolecular Architecture
-  Introduction to Biology

### Scientific Meeting Organised

-  Member of organising team, "Machine Learning for Science: Symposium and Discussion Meeting" Held in Nov 2019, IIIT Hyderabad

## Miscellaneous Experience (continued)

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- Member of organising team, INDO-GERMAN Workshop on "Computing in Chemistry, Biology and Medicine" Held in Nov 2017, IIIT Hyderabad.
- Member of organising team, CCPM Workshop 6 "Conversation with Experimentalists" held in Feb 2016, IIIT-Hyderabad.

### Other Projects

- Effect of cosolvent on protein un-folding (U/F), International Institute of Information Technology (IIIT), Hyderabad, India (Not published).**

Authors - Rohit Modee and Prof. U. Deva Priyakumar

We studied thermal denaturation and reversible U/F equilibrium of trpzip1 monomeric  $\beta$ -hairpin protein in binary (water + urea) and ternary (water + urea + TMAO) solution. We performed all-atom replica exchange MD (REMD) simulations. Results show that hydrogen bonds play an important role in forming a  $\beta$ -hairpin structure, along with van der Waals (vdW) interactions. We found disruption of intramolecular hydrogen bonds in the presence of urea.

## References

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- Prof. U. Deva Priyakumar**  
Professor & HOD,  
Center for Computational Natural Sciences and Bioinformatics (CCNSB),  
International Institute of Information Technology (IIIT),  
Gachibowli, Hyderabad-500032, India.  
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- Dr. Kavita Joshi**  
Principal Scientist,  
Physical and Materials Chemistry Division,  
CSIR-National Chemical Laboratory,  
Pune - 411008, India.  
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- Prof. Abhijit Mitra**  
Professor (Retired),  
Center for Computational Natural Sciences and Bioinformatics (CCNSB),  
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- Prof. Gopalakrishnan Bulusu**  
Adjunct Professor at IIIT-Hyderabad,  
Consultant at TCS Research,  
Adjunct Professor at Dr. Reddy's Institute of Life Sciences (DRILS),  
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