Rohit Modee.

International Institute of Information Technology (IIIT-H), Hyderabad - 500 032, India
rohit.m@research.iiit.ac.in @RohitModee Rohit Modee
rohit.modee@gmail.com https://rohitmodee.github.io/

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 in 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

1. **R. Modee**, S. Mehta, S. Laghuvarapu, and U. D. Priyakumar, "OptNet: Autonomous Molecular Geometry Optimization Using Multi-Agent Reinforcement Learning", (2023), in press.
2. **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).
3. 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).
4. **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).
5. **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

Languages	Reading, writing and speaking competencies for English, Hindi and Marathi. Speaking competencies for Telugu and Kannada.
Coding	Python, R, PyTorch, LaTeX, Basic knowledge C/C++, Perl, Bash, UNIX.
Scientific Tools	RDKit, ASE, CHARMM & CHARMM-GUI, NAMD, Gaussian & GaussView, Packmol, VMD, Avogadro.
Databases	Basic knowledge of MySQL, SQLite.
Web Dev	HTML, CSS, JavaScript, Apache Web Server.
Misc.	Academic research, teaching, training, and consultation.

Conferences

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."

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."

Conferences (continued)

- **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

- **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

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**
- **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.**

Miscellaneous Experience (continued)

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 β-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 β-hairpin structure, along with van der Waals (vdW) interactions. We found disruption of intramolecular hydrogen bonds in the presence of urea.

References

- **Prof. U. Deva Priyakumar**
  Professor & HOD,
  Center for Computational Natural Sciences and Bioinformatics (CCNSB),
  International Institute of Information Technology (IIIT),
  Gachibowli, Hyderabad-500032, India.
  deva@iiit.ac.in

- **Prof. Abhijit Mitra**
  Professor (Retired),
  Center for Computational Natural Sciences and Bioinformatics (CCNSB),
  International Institute of Information Technology (IIIT),
  Gachibowli, Hyderabad-500032, India.
  abi_chem@iiit.ac.in, and abichem@gmail.com

- **Prof. Gopalakrishnan Bulusu**
  Adjunct Professor at IIIT-Hyderabad,
  Consultant at TCS Research,
  Adjunct Professor at Dr. Reddy's Institute of Life Sciences (DRILS),
  Head, Academic Programs, iHub-Data,
  Gachibowli, Hyderabad-500032, India.
  gopal@iiit.ac.in