RONIT SARANGI

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PROFESSIONAL SUMMARY

Computational scientist with expertise in molecular modeling, quantum chemistry, and machine learning for biomolecular systems. Experienced in developing scalable workflow combining hybrid quantum/classical (QM/MM) calculations, molecular dynamics and data-driven models to predict molecular and spectroscopic properties in complex environments. Interested in applied scientist and computational modeling roles in scientific software, pharmaceutical research, and molecular machine learning.

EDUCATION

PhD Candidate, University of Southern California **Aug 2018-Aug 2023**
Advisor: Prof Anna I. Krylov.
Thesis: *Computational Spectroscopy in Gas and Condensed Phases*

Integrated BS-MS, Indian Institute of Science Education and Research, Kolkata **Aug 2012-May 2017**
Advisor: Prof. Amlan K. Roy
Masters's Thesis: *Information entropy studies in double-well and central potentials*

RESEARCH EXPERIENCE

Postdoctoral Researcher, Syracuse University **Sep 2023-Present**
Advisor: Prof. Atanu Acharya *Syracuse, NY*

- Developed machine learning models for predicting redox properties in protein cofactors using physics-inspired features and hybrid training strategies
- Designed and benchmarked excited-state force field parameterization protocol using ffTK-ORCA interface
- Created a database for redox properties for multiple protein systems and cofactors

Graduate Research Assistant, University of Southern California **Aug 2018-Aug 2023**
Advisor: Prof. Anna I. Krylov *Los Angeles, CA*

- Benchmarked and recommended basis sets for core-ionization and core-excitation calculations
- Developed a general protocol to study linear and non-linear spectra of small anions in water bulk and interface. Worked closely with experimental groups to direct experimental systems.
- Led STRUMPACK integration with Q-Chem, added optimized tensor contractions and tensor compression skills.

Research Assistant, Indian Institute of Science Education and Research **Aug 2017-Mar 2018**
Advisor: Prof. Amlan K. Roy *Kolkata, West Bengal, India*

- Worked on imaginary time propagation methods for confined systems
- Wrote and developed code to obtain ground state energies for custom potentials in Mathematica and C++.

RELEVANT PUBLICATIONS

R. Sarangi, M. L. Vidal, S. Coriani and A. I. Krylov. "On the basis set selection for calculations of core level states: Different strategies to balance cost and accuracy". *Molecular Physics* 118 (19-20), e1769872. 2020

R. Sarangi, K. D. Nanda and A. I. Krylov. "Charge-transfer-to-solvent states provide a sensitive spectroscopic probe of the local solvent structure around anions". *Molecular Physics*, e2148582. 2022

R. Sarangi, K. D Nanda, A. I. Krylov. "Two-and one-photon absorption spectra of aqueous thiocyanate anion highlight the role of symmetry in the condensed phase". *Journal of Computational Chemistry* 45 (12), 878-885. 2024

R. Sarangi, S. Maity, A. Acharya. "Machine learning approach to vertical energy gap in redox processes R Sarangi, S Maity, A Acharya". *Journal of Chemical Theory and Computation* 20 (15), 6747-6755. 2024

S. C. Mandal, **R. Sarangi**, A. Acharya. "Impact of native environment in Multiheme-Cytochrome chains of the MtrCAB complex". *Journal of Chemical Information and Modeling* 65 (9), 4568-4575. 2025

S. Maity, **R. Sarangi**, A. Acharya. "Effects of conformational sampling on computing redox properties using linear response approach". *The Journal of Physical Chemistry B* 129 (29), 7465-7474. 2025

P. O. Roy, M. Fu, **R. Sarangi**, A. I. Krylov, T. A. Wesolowski. "Can Semilocal Approximations to the Embedding Potential Tackle Charge-Transfer-to-Solvent Excitations? An Aqueous Thiocyanate Example". *Journal of Chemical Theory and Computation* 21 (20), 10452-10465. 2025

TECHNICAL SKILLS

Programming	Python, C++, tcl
Machine Learning	Scikit-learn, PyTorch, Tensorflow, feature engineering
Molecular Simulation	QM/MM simulations, force field parameterization, enhanced sampling
Software	Q-Chem, ORCA, NAMD, GROMACS, VMD
Scientific Computing	HPC workflows, STRUMPACK, Git

PRESENTATIONS

- CTTS states provide a sensitive spectroscopic probe of local structure around solute. **10th Triennial conference on Molecular Quantum Mechanics** (Blacksburg, VA, 2022)
- Machine learning approach to linear response theory for redox properties. **Mid-Atlantic Regional Meeting** (University Park, PA, 2024)
- Machine learning approach to linear response theory for redox properties. **American Chemical Society Fall** (San Diego, CA, 2025)
- Excited State Force Field Parameterization Using ffTK-Q-Chem Interface. **American Chemical Society Spring** (Atlanta, GA, 2026)

AWARDS AND GRANTS

ACCESS Computational Resources Grants **2022-Present**

- $>$ 2 million CPU hours and GPU allocations in San Diego Supercomputing Center Expanse
- Projects: Large scale simulations of Biomembranes and Proteins and ML training

Summer Research Fellowship, Indian Academy of Sciences **May 2015-Aug 2015**

- 3 months summer project in Bhabha Atomic Research Center with Prof. Swapan K. Roy
- Project: Energy pathway of simple Diels-Alder reaction

Innovation in Science Pursuit for Inspired Research (INSPIRE fellowship) **Aug 2012-May 2017**

- Awarded by Department of Science and Technology, India for 5 year BS-MS program