Ari Pereira

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Education

Stony Brook University 2023 – present
PhD in Chemistry, Advisor: Benjamin G. Levine *Stony Brook, USA*

Birla Institute of Technology and Science, Pilani - Goa Campus 2018 – 2023
Dual Degree - M.Sc Chemistry , B.E Electrical and Electronics Engineering *Goa, IN*

Research Experience

University of Southern California Los Angeles, USA (remote)
BE Thesis in EEE, Advisor: Oleg Prezhdo *Jan – May 2023*

- Used unsupervised machine learning to study the properties of Lead Halide Perovskites.
- Used mutual information to study the impact that grain boundaries have on the importance of certain geometric features in a Cesium Lead Bromide system.

Institut de Chimie Physique, Université Paris-Saclay Orsay, FR(remote)
MSc Thesis in Chemistry, Advisor: Federica Agostini *June – December 2022*

- Worked on coupled-trajectory methods based on the exact factorization for non-adiabatic dynamics.
- Studied the ultrafast isomerisation of a retinal model in an environment and the exchange of energy between reactive and vibrational modes.
- Empirically found the time complexity of different algorithms on increasing accuracy or system size.

Institut de Chimie Physique, Université Paris-Saclay Orsay, FR (remote)
Summer Internship *May 2021 – July 2021*

- Compared the quantum decoherence effects of Coupled Trajectory Mixed Quantum-Classical algorithm with Surface Hopping and exact calculations for a variety of systems.

Süd-Chemie India Pvt. Ltd. Vadodara, IN
Summer Internship *May – June 2020*

- Explored analytical tools to study catalytic converters.
- Proposed using XANES, EXAFS and XPS to study their oxidation state and structure.
- Worked under Dr Joseph Raj, Chief Manager R&D.

Publications

1. **A. Pereira**, J. Knapik, A. Chen, et al. Quantum molecular dynamics simulations of the effect of secondary modes on the photoisomerization of a retinal chromophore model. Eur. Phys. J. Spec. Top. 232, 1917–1933 (2023)

Oral & Poster Presentations

1. **A. Pereira**, A. Mehmood, B. G. Levine, "Unravelling Excited-State Twisting of Amyloid Stain Thioflavin-T: Theoretical Insights" Stony Brook University Chemistry Research Day, Stony Brook, NY, Dec 2023 (Poster)

Teaching Experience

Department of Chemistry, Stony Brook University Stony Brook, USA
Teaching Assistant

- Fall 2023: General Chemistry I
- Spring 2023: General Chemistry II

Technical Skills

Languages: Python, Fortran, C/C++, LaTeX, Bash
Algorithms: TAB, CT-MQC, Tully Surface Hopping, Ehrenfest
Instrumentation: FTIR, UV-Vis spectrophotometer, XRD, NMR, Analog Electronics Laboratory

Personal Information

Indian Citizen
Pronouns: he/him/his
Languages: English(native), Hindi, French(basic), Konkani(basic)

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