Ari R. X. Pereira

ari.pereira@stonybrook.edu | LinkedIn | Google Scholar

Education

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

- Concentration in Theoretical Chemistry

Birla Institute of Technology and Science, Pilani - Goa Campus — Goa, IN
Double Degree — *2018-2023*

- Integrated M.Sc in Chemistry (First Division)
- B.E in Electrical and Electronics Engineering (First Division)

Research Experience

Stony Brook University — Stony Brook, NY
Department of Chemistry and Institute for Advanced Computational Science — *June 2023-present*

- Advisor: Benjamin G. Levine
- Worked on developing novel nonadiabatic dynamics methods to simulate ultrafast photochemistry involving dense electronic states.

University of Southern California — Los Angeles, CA (remote)
Department of Chemistry — *Jan – May 2023*

- Advisor: Oleg V. Prezhdo
- Performed research work for senior year thesis in Electrical Engineering.
- Used unsupervised machine learning to study the properties of Lead Halide Perovskites.
- Used mutual information to study the impact that grain boundaries have on certain geometric features in a Cesium Lead Bromide system.

Université Paris-Saclay — Orsay, France(remote)
Institut de Chimie Physique CNRS — *June – December 2022*

- Advisor: Federica Agostini
- Performed research work for senior year thesis in Chemistry.
- 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.

Université Paris-Saclay — Orsay, France (remote)
Institut de Chimie Physique CNRS — *May 2021 – July 2021*

- Advisor: Federica Agostini
- Performed summer research work in theoretical Chemical Physics.
- 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, India
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. R. X. Pereira** and B. G. Levine "Approximate Pointer States for Nonadiabatic Dynamics" Nonadiabatic dynamics, electron-phonon interactions, and spin-phonon couplings, Princeton Center for Theoretical Science, Princeton, NJ, April 2025 (Poster)

2. **A. R. X. Pereira** and B. G. Levine, "A Pointer Basis for Molecular Dynamics on Many Electronic States" Stony Brook University Chemistry Research Day, Stony Brook, NY, Oct 2024 (Poster)

3. **A. R. X. Pereira**, A. Mehmood, B. G. Levine, "Unraveling 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 2024: General Chemistry II

Technical Skills

Languages: Python, Fortran, C/C++, LaTeX, Bash
Methods: DFT, MP2, CAS, TAB, CT-MQC, Tully Surface Hopping, Ehrenfest
Software: Matlab, psi4, TeraChem

Personal Information

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

Updated May 3, 2025