Ari Pereira

f20180946@goa.bits-pilani.ac.in | LinkedIn | aripereira.github.io

Research Interests

Theoretical Chemistry, Excited State Dynamics, Quantum Computing

Education

Birla Institute of Technology and Science, Pilani - Goa Campus 2018 – 2023 (expected)
Dual Degree - M.Sc (Hons.) Chemistry , B.E (Hons.) Electrical and Electronics Engineering *Goa, IN*
Current CGPA: 7.37

Experience

Institut de Chimie Physique, Université Paris-Saclay Orsay, FR
Research Intern *May 2021 – Present*

- Working on ultra-fast non-adiabatic dynamics with Dr Federica Agostini
- Comparing the Coupled Trajectory Mixed Quantum-Classical algorithm with Surface Hopping and exact calculations for a variety of systems
- A second line of work is accounting for a classical laser field explicitly in the simulations to simulate both the excitation and the dynamics after scattering

Süd-Chemie Vadodara, IN
Summer Research Intern *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

Projects

Solutions to the Ornstein-Zernike Equation | *Supervisor: Prof R.N Behera* Jan 2020 – June 2020

- The project covered an introduction to statistical mechanics
- Studied different methods to solving an integral equation for ideal liquids
- Studied two closure relations: the Percus–Yevick approximation, and the Hypernetted-chain equation

Biosensor Modeling | *Supervisor: Dr Gautam Bacher* August 2021 – Present

- Modeling different channel materials in electric double layer transistors

Selected Coursework

Chemistry: Introduction to Quantum Chemistry, Quantum Chemistry and Group Theory, Chemical Kinetics and Liquid Theory, Thermodynamics, Instrumental Methods of Analysis, Inorganic Chemistry I, II & III

Mathematics: Probability and Statistics, Ordinary Differential Equations, Linear Algebra and Complex Variables, Vector Calculus

Physics: Electromagnetic Theory, Mechanics Oscillations and Waves

Engineering: Computer Programming, Thermodynamics, Digital Design, Electronic Devices, Microelectronics, Signals & Systems, Control Systems

Technical Skills

Languages: Fortran, Python, C/C++, LaTeX, Bash
Developer Tools: Git, VS Code, Visual Studio, Unix
Algorithms: CT-MQC, FSSH, Ehrenfast, Exact Dynamics

Personal Information

Indian Citizen
Languages: English(native), Hindi, French(basic), Konkani(basic)

Updated Aug 2021