Rahul Raj K

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https://github.com/Razer-07

Integrated BS-MS, Chemistry, IISER- Kolkata

Education

Indian Institute of Science Education and Research, Kolkata
5-year BS-MS dual degree *August 2017- July 2022*
Major in Chemistry & Minor in Physics
GPA: 3.206/4

Research Interests

Quantum Chemistry, Computational Chemistry, Machine Learning

Skills

Languages: **Python**, MATLAB, LaTeX,C(basic level)

Software/Packages: Gaussian, Git/Github, LONDON (quantum chemistry software), Orca, TheoDORE, Multiwfn, IBM Qiskit, Origin Pro, GNU Plot, Office

Operating Systems: Particularly interested in Linux OS, Mac OS, Windows OS
Worked with **supercomputer**(Dirac) as a part of Master's Thesis at IISER Kolkata for the computation with quantum chemistry software

standard markup language: HTML
stylesheet language: CSS

Experience and Research Projects

- **Computing Electronic Spectra of Molecules in Strong Magnetic Fields Using Time Dependent Hartree-Fock (TDHF)**
  Supervisor: Prof. Sangita Sen *May 2021 - May 2022*

  In the **masters thesis** project at Indian Institute of Science Education and Research Kolkata, electronic state energies of the H_2O, H_2 molecule and He atom were computed and plotted under strong magnetic fields using the linear response of Hartree-Fock theory with the aid of the computational chemistry software called LONDON. Additionally,also computed the spectral intensities to explore how the symmetric forbidden transitions become allowed in the presence of magnetic fields that lift this symmetry. I try to justify the changes in the electronic spectra at the level of orbital changes due to the magnetic field by plotting orbital density of molecules under the influence of a strong magnetic field.
  Project : link.

- **Numerical Problems in Quantum Chemistry**
  Supervisor: Dr. Erik Tellgren *January 2023 - February 2023*

  Worked on a remote project under the guidance of Dr.Erik Tellgren at OSLO University, Norway. As a remote project member, I was engaged in a project related to method development and numerical problems in quantum chemistry using PySCF. My work so far has included successfully computing the Fock matrix for H_2 and implementing fixed-point iteration for the Hartree-Fock algorithm using PySCF. Discontinued after joining IISER to continue MS thesis research

- **Computing Electronic Spectra of Molecules in Strong Magnetic Fields Using Time Dependent Hartree-Fock (TDHF)**
  Supervisor: Prof. Sangita Sen *February 2022 - Present*

This research builds upon my Master's thesis, focusing on the utilization of Natural Transition Orbitals (NTOs) to analyze and visualize electronic excitations in the presence and absence of an applied field.

- **Time-Dependent Quantum Chemistry Calculations**
  Supervisor: Prof. Ashwani Kumar Tiwari *December 2019 - January 2020*

  Winter Project at Indian Institute of Science Education and Research, Kolkata

  A winter reading project in quantum chemistry, where I solved problems related to particles in a box with different lengths.

- **Statistical Mechanics-Quantum Formalism**
  Supervisor: Prof. Subhasis Sinha *May 2019-July 2019*

  Summer project at Indian Institute of Science Education and Research , Kolkata
  A reading project in physics on the topic of the formulation of quantum statistics in statistical mechanics, using the book "Statistical Mechanics" by R.K Pathria. I solved problems involving quantum-mechanical ensemble theory. By completing this project, I have gained a deep understanding of the principles of statistical mechanics and quantum mechanics, and their application to quantum-mechanical systems.

- **Read Introduction to Real Analysis**
  Supervisor: Prof. Noufal Asharaf *Jun 2018-July 2018*

  Summer Project at CUSAT, Kerala

  A reading project in mathematics that covered the topics of sequences, series, and limits in the book "Introduction to Real Analysis" by Robert G. Bartle and Ronald R. Sherbert.

Course Projects

Wave Function Animation
Instructor: Prof. Soumitro Banerjee *August 2021–Dec 2021*

Solved the wavefunction for different potentials and created animation of $|\Psi|^2$.
For the complete project: Click Here

Other Projects

Time series analysis of Tesla stock

Created a time series analysis of Tesla stock for a duration of 1-year using python programming language. Click here

Online Payments Fraud Detection using Python & ML

Using the credit card dataset from Kaggle predicts whether a transaction is a fraud using python programming language. Click here

Relevant Courses

- **Quantum Chemistry I** Quantum Chemistry I
- **Quantum Chemistry II**Quantum Chemistry II
- **Advanced Quantum Chemistry** Advanced Quantum Chemistry
- **Computational Chemistry** Computational Chemistry
- **Statistical Thermodynamics** Statistical Thermodynamics
- **Applications of Chemical Thermodynamics** Applications of Chemical Thermodynamics
- **Group Theory and Spectroscopy** Fundamentals of Spectroscopy
- **Group Theory and Spectroscopy** Group Theory and Spectroscopy
- **Physics IV** Physics IV
- **Intermediate Quantum Mechanics** Intermediate Quantum Mechanics
- **Advanced Quantum Mechanics** Advanced Quantum Mechanics
- **Chemistry of Transition Elements** Chemistry of Transition Elements
- **Linear Algebra I** Linear Algebra I
- **Analysis I** Analysis I
- **Analysis II** Analysis II
- **Probability I** Probability I
- **Introduction to Programming (Python)** Introduction to Programming (Python)

Other Certificate

- **Supervised Machine Learning: Regression and Classification** Certificate
- **Qubit by Qubit's Introduction to Quantum Computing course with IBM Quantum.**

  A two semester course of "Introduction to Quantum Computing" (including Fundamentals of Quantum Computing, Applications of Quantum Computing, Quantum Finance, Quantum Chemistry) Certificate

Awards & Achievements

- Selected for attending **Vijyoshi**-National Science Camp in 2017.
- Awarded INSPIRE Fellowships during graduate studies(2017-2022)
- Belonged to the **top 1%** of students who passed the All India Senior Secondary Examination in 2017
- Secured all India Rank 321 in IISER Aptitude Test(IAT) in 2017
- Secured Kerala Engineering Architecture Medical (KEAM) rank (general)1016, and OBC rank 350 out of 90,806 candidates
- Accepted to Qubit by Qubit's Introduction to Quantum Computing course sponsored by IBM Quantum with a Full Scholarship for Semester 1 & Semester 2 (September - April 2023)

Activities

- Webinar on Quantum Computing of Quantum Computing by Prof. David Jamieson, The University of Melbourne Click here
- webinar in engineering (India's Largest), Professor of MIT will be presenting on the topic of - AI, 3D Printing, Chemical Metallurgy, and Entrepreneurship Click here
- International Conference on recent trends in chemistry of Materials 2021(ICRTCM 2021)Click here

- Webinar in the field of Business Administration and Finance (Forethought India) Click here
- Attended Intersection of Theory and Computation in Chemistry(ITCC) conference held on 1st July at IISER Kolkata Click here
- Poster presentation as part of master's project evaluation in front of whole department Click here

Other Interests

Coding/Competitive Programming, Computer Gaming, Football, Badminton, Table Tennis.