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AAMOD ATRE

B.E. | Major - Chemical Engineering | Minor - Physics

About Me

1. **INTERESTED** in understanding molecular interactions in materials & their dynamics across various timescales
2. **BELIEVE** in approaching a problem theoretically prior to pursuing computational and experimental study
3. **INTEND** to pursue the development of theoretical frameworks of atomic, molecular and optical sciences

Education History

Undergraduate	**Birla Institute of Technology and Science, Pilani**	**Aug 2017 - Aug 2021**
GPA 8.65/10.0	B.E (Hons.) Chemical Engg. | Minor : Physics	
Higher Secondary	**FIITJEE Junior College, Kukatpally, Hyderabad**	**Apr 2015 - Aug 2017**
Percentage : 96.5 %	Grades XI & XII	
Senior Secondary	**Delhi Public School, Nacharam, Hyderabad**	**Mar 2013 - Mar 2015**
GPA : 10.0/10.0	Grades IX & X	

Work Experience

Remote Research Assistantship **Oct. 2021 - Present**
Dr. Aaron Kelly | *Max Planck Institute for the Structure and Dynamics of Matter, Hamburg*
Studying the cavity-modified molecular dynamics with spin-mapping-based semiclassical techniques.

Remote Research Internship **July. 2021 - Sept. 2021**
Dr. Pengfei Huo | *University of Rochester, New York*
Compared the performance of standard and spin-based partially linearized density matrix (PLDM) algorithms in calculating linear absorption spectra of a bi-exciton coupled dimer model.

Undergraduate Thesis | Research Internship **Jan. 2021 - June 2021**
Dr. Jeremy Richardson | *ETH Zürich*
Gauged the efficacy of a spin-mapping-based semiclassical dynamics technique by studying the population and coherence dynamics of exciton relaxation in a 1D polymer chain. Formulated a spin-mapping for tight-binding polymer chains which conform to SU(*2*) symmetry.

Research Internship **May 2019 - July 2019**
Prof. Bibek Dash | *CSIR Institute of Minerals and Materials Technolgy, India*
DFT-based computational designing of triazole-based molecular precursors for selective CO_2 capture. Statistically determined the optimum functional-basis combination to model the CO_2-triazole interactions with DFT. Studied CO_2 interactions with the aromatic building blocks to propose a new triazole moiety design.

Technical Skills

Programming	**Software Packages**		**Language**
Python	MATLAB	LAMMPS	English (Native/Bilingual)
Fortran	Maple	Quantum Espresso	German (Elementary)
C	Mathematica	Gaussian 09	French (Elementary)
			Marathi | Hindi (Native)

Undergraduate Teaching Experience

Teaching Assistant **Aug. 2020 - Dec. 2020**
Dr. S. D. Manjare | *Process Design Principles - I*

Teaching Assistant **Aug. 2020 - Dec. 2020**
Dr. Radhika Vathsan | *Quantum Mechanics - II*

Standardized Tests

GRE General Test : 335/340 | Quant : 168/170 | Verbal : 167/170 | Analytical Writing : 5/6 **Aug. 2021**
TOEFL : 115/120 | Reading : 30/30 | Listening : 30/30 | Speaking : 25/30 | Writing : 29/30 **Sept. 2021**

Academic Interests

1. Dynamics of many-body, optical and open quantum systems.
2. Development of theoretical and computational chemistry.
3. *Ab initio* molecular modelling and statistical physics.

Relevant Academic Credit Courses

Quantum Mechanics I & II	Solid State Physics	Statistical and Molecular thermodynamics
Statistical Mechanics	Atomic and Molecular Physics	Transport Phenomenon
Nonlinear Dynamics and Chaos Theory		

Featured Undergraduate Projects

Designing Lithium-based metal organic frameworks for hydrogen production **Jan. 2020 - June 2021**
Design Project | *Dr. Paramita Haldar*

Ab initio computational study of graphene-based Li-MOFs, employing density functional theory implementation in Quantum Espresso for electronic structure calculations & reactive molecular dynamics within LAMMPS framework to study hydrogen evolution amongst proposed models.

Study of cavity QED formalism and modern quantum control techniques **Aug. 2020 - Dec. 2020**
Study Project | *Dr. Raghunath Ratabole*

Literature survey of modern qubit implementations, entangled state preparation and quantum gate implementations in molecule-coupled cavity systems. Study of field quantization, cavity QED formalism and the applications of Jaynes-Cummings model.

Modelling kinetics of photo-catalytic reactions involved in waste-water treatment **Aug. 2019 - Dec. 2019**
Study Project | *Dr. Sharad Sontakke*

Modelled TiO_2-based photocatalytic degradation of phenol and extraction of Cr and Cu ions with MATLAB. Optimizated TiO_2 catalyst concentration and reaction rates for varying contamination levels.

Study of metal-organic frameworks as tools for adsorptive CO_2 capture **Jan. 2019 - May. 2019**
Study Project | *Dr. Richa Singhal*

Literature review of thermodynamic and electronic properties of MOFs. Studied the methodologies and developments in the field of CO_2 capture, focusing on MOFs.

Other Academic Projects **Aug. 2018 - Dec. 2020**
BITS Pilani

· Simulation of Hamiltonian maps and transport in structured fluids
· Fugacity coefficient estimation of pure CO_2 and H_2O using Van der Waals and Soave-Redlich-Kwong EOS modelling
· Derivation of various thermodynamic relations for a grand canonical ensemble of NO_2

Extracurricular Activities

Quantum Computing	· Cleared Quantum Open Source Foundation (QOSF) cohort 4 assesment task	**Sept. 2021**
	· Completed IBM Quantum's Global Summer School	**June 2020**
Positions of Responsibility	· Core Member : *Kala - Fine Arts Club*	**Mar. 2018 - May 2020**
Hobbies	· Long distance running, swimming and squash sports	
	· Avid reader of fiction and non fiction literature	