

AAMOD ATRE

B.E. (Hons.) | 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 GPA 8.65/10.0	Birla Institute of Technology and Science, Pilani B.E (Hons.) Chemical Engg. Minor : Physics	Aug 2017 - Aug 2021
Higher Secondary Percentage : 94.7 %	FIITJEE Junior College, Kukatpally, Hyderabad Grades XI & XII	Apr 2015 - Aug 2017
Senior Secondary GPA : 10.0/10.0	Delhi Public School, Nacharam, Hyderabad Grades IX & X	Mar 2013 - Mar 2015

Work Experience

Remote Research Assistantship **Sept. 2021 - Present**

Dr. Aaron Kelly | Max Plank 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 Technology, India

DFT-based computational designing of triazole-based molecular precursors for selective CO₂ capture. Statistically determined the optimum functional-basis combination to model the CO₂-triazole interactions with DFT. Studied CO₂ interactions with the aromatic building blocks to propose a new triazole moiety design.

Technical Skills

Languages

Programming	Software Packages		Languages
Python	MATLAB	LAMMPS	English (Native/Bilingual)
Fortran	Maple	Quantum Espresso	German (A1)
C	Mathematica	Gaussian 09	French (A2)
			Marathi Hindi (Native)

Undergraduate Teaching Experience

Teaching Assistant **Aug. 2020 - Dec. 2020**

Dr. Radhika Vathsan | Quantum Mechanics - II

Teaching Assistant **Aug. 2020 - Dec. 2020**

Dr. S. D. Manjare | Process Design Principles - I

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 Statistical Mechanics Nonlinear Dynamics and Chaos Theory	Solid State Physics Atomic and Molecular Physics	Statistical and Molecular thermodynamics Transport Phenomenon
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Featured Undergraduate Projects

1	Design Project <i>Jan 2020 - June 2021</i> Dr. Paramita Halder BITS Pilani	Ab initio design of Lithium-based metal organic frameworks (Li-MOFs) for hydrogen production <ul style="list-style-type: none">· Employing DFT to develop the theoretical model of a graphene-based Li-MOF.· Employing classical molecular dynamics to gauge the hydrogen evolution potential of the proposed model.
2	Study Project <i>August 2020 - Dec 2020</i> Dr. Raghunath Ratabole BITS Pilani	Study of the cavity QED formalism and modern quantum control techniques. <ul style="list-style-type: none">· Study of cavity QED formalism and the applications of Jaynes-Cummings model.· Literature survey of modern qubit implementations, entangled state preparation and quantum gate implementations in molecule-coupled cavity systems.
3	Study Project <i>Aug 2019 - Dec 2019</i> Dr. Sharad Sontakke BITS Pilani	Modelling kinetics of photocatalytic reactions involved in waste-water treatment <ul style="list-style-type: none">· Modelling TiO_2-based photocatalytic degradation of phenol and extraction of Cr and Cu ions with MATLAB.· Optimization of TiO_2 catalyst concentration and reaction rates for varying contamination levels.
4	Study Project <i>Jan 2019 - May 2019</i> Dr. Richa Singhal BITS Pilani	Study of metal-organic frameworks as tools for adsorptive CO_2 capture <ul style="list-style-type: none">· Literature review of thermodynamic and electronic properties of MOFs.· Studying the methodologies and developments in the field of CO_2 capture.
5	Other Academic Projects <i>Aug 2018 - Dec 2021</i> BITS Pilani	<ul style="list-style-type: none">· Simulation of Hamiltonian maps and transport in structured fluids.· Fugacity coefficient estimation of pure CO_2 and water for comparative study using Van der Waals and Soave-Redlich-Kwong EOS modeling.· 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 : <i>Kala - Fine Arts Club</i>	Mar. 2018 - May 2020
Hobbies	· Long distance running, swimming and squash sports · Avid reader of fiction and non fiction literature	