## AAMOD ATRE

In Pursuit | M. Sc. Quantum Science and Technology

#### **About Me**

- 1. INTERESTED in understanding molecular and optical interactions & their dynamics across various timescales
- 2. ENJOY delving into the theoretical underpinnings of a problem and exploring the system computationally
- 3. INTEND to pursue the development of theoretical frameworks in atomic, molecular and optical sciences

Technical University of Munich	Oct 2022 - Present
M. Sc. Quantum Science and Technology	
Birla Institute of Technology and Science, Pilani	Aug 2017 - Aug 2021
B.E. Chemical Engg.   Minor : Physics	
FIITJEE Junior College, Kukatpally, Hyderabad	Apr 2015 - Aug 2017
Grades XI & XII	
Delhi Public School, Nacharam, Hyderabad	Mar 2013 - Mar 2015
Grades IX & X	
	M. Sc. Quantum Science and Technology  Birla Institute of Technology and Science, Pilani B.E. Chemical Engg.   Minor : Physics  FIITJEE Junior College, Kukatpally, Hyderabad  Grades XI & XII  Delhi Public School, Nacharam, Hyderabad

### Work Experience

Student Assistant | HiWi April. 2023 - Present

Dr. Peter Rabl | Walther Meißner Institute, Munich

Working towards improving cascading quantum networks' simulations.

#### Remote Research Assistantship

Oct. 2021 - Oct. 2022

Dr. Aaron Kelly | Max Planck Institute for the Structure and Dynamics of Matter, Hamburg

Benchmarked a semiclassical mapping-based dynamics method (spin-PLDM) by modelling the interactions between an atomic subsystem and cavity-modified field modes.

## 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			Language
Programming	Softwa	re Packages	English (Native/Bilingual)
Python	MATLAB	LAMMPS	German (Elementary - A2)
Fortran (Elementary)	Maple	Quantum Espresso	French (Elementary)
C (Elementary)	Mathematica	Gaussian 09	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
<b>TOEFL</b> : 115/120   Reading: 30/30   Listening: 30/30   Speaking: 25/30   Writing: 29/30	Sept. 2021

#### **Academic Interests**

- Dynamics of many-body, optical and open quantum systems.
- Development of techniques in theoretical and computational chemistry.
- 3. Development of molecular and optical tools towards quantum technology.

Relevant Undergraduate Credit Courses			
Quantum Mechanics I & II	Solid State Physics	Statistical and Molecular	
Statistical Mechanics	Atomic and Molecular Physics	thermodynamics	
Nonlinear Dynamics and Chaos		Transport Phenomenon	
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 Study Project | Dr. Raghunath Ratabole

Aug. 2020 - Dec. 2020

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.

<b>Extracurricular Activities</b>		
Quantum Computing	· Cleared Quantum Open Source Foundation (QOSF) cohort 4 assesment task	Sept. 2021
	· Completed IBM Quantum's Global Summer School	June 2020, July 2022
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	

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