

## AAMOD ATRE

Birla Institute of Technology and Science, Pilani - Goa, India  
B.E. (Hons.) | Major - Chemical Engineering Minor - Physics | CGPA : 8.65

Programming Languages	Software Packages	In Training
Python 3 C C++	Gaussian 09 Quantum Espresso Avogadro COMSOL MATLAB Maple AutoCAD Adobe Photoshop	LAMMPS Mathematica Fortran

### Relevant Academic Credit Courses

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

### About Me

- INTERESTED** in understanding materials and their interactions at an atomic level and exploring the various dynamics that emerge.
- BELIEVE** in approaching a problem theoretically prior to pursuing computational and experimental study.
- INTEND** to pursue theoretical chemistry and chemical physics to investigate the study of various quantum phenomenon.

### My Interests

- Dynamics of many-body and open quantum systems.
- Methods in theoretical and computational chemistry.
- Ab-initio molecular modelling and non-equilibrium statistical processes.

### Featured Projects and Work Experience

1	<b>Research Internship</b> <i>July 2021 - August 2021</i> Dr. Pengfei Huo University of Rochester (Virtually Conducted)	<b>Modelling linear absorption spectroscopy with partially linearized density matrix (PLDM) methods</b> <ul style="list-style-type: none"><li>Study of principles of linear and non-linear spectroscopy.</li><li>Implementing a bi-exciton coupled dimer model.</li><li>Comparison of linear spectra determined by standard PLDM and spin-based PLDM techniques.</li></ul>
2	<b>Undergraduate Thesis</b> <i>Jan 2021 - June 2021</i> Dr. Jeremy Richardson ETH Zurich	<b>Modelling nonadiabatic dynamics in conjugated polymer chains with quasiclassical spin-based mapping techniques.</b> <ul style="list-style-type: none"><li>Employed a generalised spin-based mapping approach to study exciton relaxation dynamics in polymer chains.</li><li>Formulated an <math>SU(2)</math>-based technique suitable to model exciton dynamics tight-binding polymer chains.</li></ul>
3	<b>Design Project</b> <i>Jan 2020 - June 2021</i> Dr. Paramita Halder BITS Pilani	<b>Ab initio design of Lithium-based metal organic frameworks (Li-MOFs) for hydrogen production</b> <ul style="list-style-type: none"><li>Literature review of hydrogen evolution reaction and techniques for modelling MOFs.</li><li>Employing DFT to develop the theoretical model of a graphene-based Li-MOF.</li><li>Employing classical molecular dynamics to gauge the hydrogen evolution potential of the proposed model.</li></ul>

## Featured Projects and Work Experience

4	<b>Study Project</b> <i>August 2020 - Dec 2020</i> Dr. Raghunath Ratabole BITS Pilani	<b>Study of the cavity QED formalism and modern quantum control techniques.</b> · Literature survey of modern qubit implementations. · Study of cavity QED formalism and the applications of Jaynes-Cummings model. · Literature survey of entangled state preparation and quantum gate implementations in molecule-coupled cavity systems.
5	<b>Research Internship</b> <i>May 2019 - July 2019</i> Prof. Bibek Dash CSIR IMMT	<b>DFT based computational designing of molecular precursors to triazole based frameworks for selective CO<sub>2</sub> capture</b> · Statistically finding the optimum functional - basis combination to model the CO <sub>2</sub> interactions with triazole frameworks. · Studying CO <sub>2</sub> interactions with the aromatic building blocks to propose a new triazole moiety design.
6	<b>Study Project</b> <i>Aug 2019 - Dec 2019</i> Dr. Sharad Sontakke BITS Pilani	<b>Modelling kinetics of photocatalytic reactions involved in waste-water treatment</b> · Literature review of heavy metal and organic matter degradation via photocatalysis. · Modelling TiO <sub>2</sub> -based photocatalytic degradation of phenol and extraction of Cr and Cu ions with MATLAB. · Optimization of catalyst concentration and reaction rates based on varying contamination levels.
7	<b>Study Project</b> <i>Jan 2019 - May 2019</i> Dr. Richa Singhal BITS Pilani	<b>Study of metal-organic frameworks as tools for adsorptive CO<sub>2</sub> capture</b> · Literature review of thermodynamic and electronic properties of MOFs. · Studying the methodologies and developments in the field of CO <sub>2</sub> capture.

## Academic References

1	<b>Prof. Bibek Dash</b>	Scientist	CSIR - Institute of Minerals and Materials Technology, Bhubaneswar, India	+91 9632166242 <a href="mailto:bibek@immt.res.in">bibek@immt.res.in</a>
2	<b>Dr. Paramita Haldar</b>	Assistant Professor	Birla Institute of Technology and Science, Pilani, Goa, India	+91 832-2580-280 <a href="mailto:paramitah@goa.bits-pilani.ac.in">paramitah@goa.bits-pilani.ac.in</a>
3	<b>Dr. Raghunath Ratabole</b>	Associate Professor	Birla Institute of Technology and Science, Pilani, Goa, India	+91 832-2580-417 <a href="mailto:ratabole@goa.bits-pilani.ac.in">ratabole@goa.bits-pilani.ac.in</a>

## Educational Details

Undergraduate University	Higher Secondary School	Secondary School
Birla Institute of Technology and Science, Pilani, Goa, India <b>Aug 2017 - Aug 2021</b>	FIITJEE Junior College Kukatpally, Hyderabad <b>Apr 2015 - Mar 2017</b>	Delhi Public School Nacharam, Hyderabad <b>Dec 2003 - May 2005</b>

## Extracurricular Activities and Hobbies

- Teaching Assistant - Quantum Mechanics II and Process Design Principles I, Fall Semester 2020.
- Completed IBM Quantum's Global summer school on Quantum Computing, 2020.
- Member of the core at the fine arts club 'Kala' at BITS Pilani, Goa Campus (2018 - 2020).
- Long distance runner and fitness enthusiast, pursuing swimming, squash, badminton sports.
- Avid reader of fiction and non-fiction literature ... whenever time permits.