LinkedIn/Aamod
aamodatre51297@gmail.com +91 78938 75280
f20170790g@alumni.bits-pilani.ac.in +91 79899 06502

AAMOD ATRE

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

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

Relevant Academic Credit Courses

Completed

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

About Me

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

My Interests

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

Featured Projects and Work Experience

1 **Undergraduate Thesis**

Jan 2021 - Present
Dr. Jeremy Richardson
ETH Zurich

Implementation and extension of quasiclassical spin-mapping approaches to model nonadiabatic dynamics in conjugated chain polymers.

· Employing a generalised spin-based mapping approach to model linear polymer chains.
· Currently studying a spin-mapping suited to linear polymer chains.

2 **Design Project**

Jan 2020 - Present
Dr. Paramita Haldar
BITS Pilani

Ab initio design of Lithium-based metal organic frameworks (Li-MOFs) for hydrogen production

· Literature review of hydrogen evolution reaction and techniques for modelling MOFs.
· 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.

3 **Study Project**

August 2020 - Dec 2020
Dr. Raghunath Ratabole
BITS Pilani

Study of the cavity QED formalism and modern quantum control techniques.

· 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.

Featured Projects and Work Experience

4	**Research Internship** *May 2019 - July 2019* Prof. Bibek Dash CSIR IMMT	**DFT based computational designing of molecular precursors to triazole based frameworks for selective CO_2 capture** · Statistically finding the optimum functional - basis combination to model the CO_2 interactions with triazole frameworks. · Studying CO_2 interactions with the aromatic building blocks to propose a new triazole moiety design.
5	**Study Project** *Aug 2019 - Dec 2019* Dr. Sharad Sontakke BITS Pilani	**Modelling kinetics of photocatalytic reactions involved in waste-water treatment** · Literature review of heavy metal and organic matter degradation via photocatalysis. · Modelling TiO_2-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.
6	**Study Project** *Jan 2019 - May 2019* Dr. Richa Singhal BITS Pilani	**Study of metal-organic frameworks as tools for adsorptive CO_2 capture** · Literature review of thermodynamic and electronic properties of MOFs. · Studying the methodologies and developments in the field of CO_2 capture.
7	**Other Academic Projects** *Aug 2018 - Dec 2021* BITS Pilani	· Simulation of Hamiltonian maps and transport in structured fluids. · Fugacity coefficient estimation of pure CO2 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

Academic References

1	**Prof. Bibek Dash**	Scientist	CSIR - Institute of Minerals and Materials Technology, Bhubaneshwar, India	+91 9632166242 bibek@immt.res.in
2	**Dr. Paramita Haldar**	Assistant Professor	Birla Institute of Technology and Science, Pilani, Goa, India	+91 832-2580-280 paramitah@goa.bits-pilani.ac.in
3	**Dr. Raghunath Ratabole**	Associate Professor	Birla Institute of Technology and Science, Pilani, Goa, India	+91 832-2580-417 ratabole@goa.bits-pilani.ac.in

Educational Details

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

Extracurricular Activities and Hobbies

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

Date: March 31, 2021 Place: Zurich, Switzerland 8053