Dr. Soumya Mukherjee

Assistant Professor, Department of Chemistry, MANIT, Bhopal
PhD in Quantum Chemistry and Quantum Dynamics
Research Topic: Quantum Chemistry and Quantum Dynamics, Computational Environmental Chemistry, Computational Medicinal Chemistry

Contact Details	
Email Id	soumyamukherjee093@gmail.com, soumya@manit.ac.in
Phone No.	+919674378580
Google Scholar	https://scholar.google.com/citations?user=nE1jofwAAAAJ&hl=en
Scopus Author ID	57672563200
Web of Science Author ID	LTD-7291-2024
Linked In	https://www.linkedin.com/in/dr-soumya-mukherjee-4483a0337/
ORCID	https://orcid.org/0009-0006-8563-920X
Vidwan	582656

Education			
Organization	**Start Date**	**End Date**	**Degree/Designation**
Indian Association for the Cultivation of Science, Kolkata	18th October, 2022	31st December, 2023	Research Associate - I
Indian Association for the Cultivation of Science, Kolkata	3rd August, 2016	17th October, 2022	Ph.D (SPM Fellow)
University of Calcutta, Kolkata	August, 2014	July, 2016	M.Sc. in Chemistry (Specialization in Physical Chemistry with 87.1% marks, ranked 2nd)
Asutosh College, Kolkata (affiliated to University of Chemistry)	July, 2011	July, 2014	B.Sc. (Hons.) in Chemistry (81.75%, ranked 4th)

PhD Details		
Organization	**Topic**	**Supervisor**
Indian Association for the Cultivation of Science, Kolkata	Non-Adiabatic Processes in Molecular Spectroscopy and Scattering	Professor Satrajit Adhikari

Subjects Taught	
U.G	CHY 107 or CHY 24110 or CY 1110: Environmental Chemistry
	CHY 125 or CHY 24126 or CY 1126: Chemistry Practical or Engineering Chemistry

	Laboratory
P.G	CHY 24533: Instrumental Methods of Analysis
	CY MS 513: Organic Chemistry I
	CHY 24518 or CY MS 518: Seminar I
	CY MS 517: Organic Chemistry Lab I
	CHY 24523: Organic Chemistry – II (Heterocyclic Compounds and Organic Reagents)
	CHY 24551: Chemical and Statistical Thermodynamics
	CHY 24528: Seminar II
	CHY 529 or CHY 24527: Organic Chemistry Lab II
	CHY 614 or CHY 24617: Chemistry Lab III or Organic Chemistry Lab III and Minor Project-III (Self learning)
	CHY 615: Seminar II
	CHY 659 or CHY 24614: Natural Products and Medicinal Chemistry

Teaching Experience				
Organization	**Start Date**	**End Date**	**Designation**	**Nature of Work**
Maulana Azad National Institute of Technology, Bhopal	10th September, 2025	Till Now	Assistant Professor Grade-II (Pay Level-11)	Teaching & Research
Maulana Azad National Institute of Technology, Bhopal	8th January, 2024	9th September, 2025	Assistant Professor Grade-II (Pay Level-10)	Teaching & Research

Project/Ph.D. Students			
Name	Type	Co-Supervisor	Research Area
Priyanka Kumari	Part Time Ph.D	Dr. Rampal Pandey	Beyond Born-Oppenheimer Theory, Computational H_2 Storage Study
Radheshyam Trivedi	Part Time Ph.D	Prof. Amit Dubey	Beyond Born-Oppenheimer Theory, Computational Atmospheric Chemistry
Manpreet Singh	Part Time Ph.D		Computational Material Chemistry
P. Ayushi Rao	Full Time Ph.D		Computational Biochemistry
Poonam Ahirwar	ANRF Project Scholar		Computational Environmental Chemistry, Molecular Docking
Mansi Sunil Parab	M.Sc. Project Student (completed on June, 2025)		Computational H_2 Storage Study
Kuldeep Nagar	M.Sc. Project Student (completed on June, 2025)		Computational Atmospheric Chemistry
Tanu	M.Sc. Project Student (started on August, 2025)		Computational Organic Chemistry
Neha Bharti	M.Sc. Project Student (started on August, 2025)		Computational Organic Chemistry

Lab Manual Preparation	
Organization	**Details**
Maulana Azad National Institute of Technology, Bhopal	Procurement of Molpro Software License (useful for various electronic structure calculations) has been done using seed grant (tender number: 2025_MANIT_795322_1).
	Extensive modifications have been done for the existing Organic Chemistry lab manual (in English) for the M.Sc. students. On the other hand, the entire lab manual has been translated into Hindi so that the document can be available in bilingual form.

Lab Details		
Device or Software	**Utilization**	**Small Picture**
Molpro Software	Electronic structure calculation, potential energy surface construction, diabatization techniques	NA
Gaussian 16 software	Electronic structure calculation, geometry optimization, molecular orbital calculations	NA

Sponsored Research Projects (Completed/Ongoing)					
Title of the Project	**Sponsoring Agency**	**Duration**	**Details**	**Amount**	**Co-PI (if any)**
In-Silico Study of Designing Eco-Friendly Reagents for Prevention of Environmental Pollutions Leading to Sustainable Development ((File No. ANRF/ECRG/2024/000810/CS dated 13th June, 2025))	ANRF, DST, India	Three years (17th June, 2025 to 16th June, 2028)	In this project, ab initio investigations, namely, calculations of optimized structure, single-point energy, dipole moment and many other properties will be performed for various atmospheric / hydrospheric reactions. Those parameters will be further used to generate adiabatic potential energy curves (PECs) / surfaces (PESs) and non-adiabatic coupling terms (NACTs) followed by diabatic PECs/PESs and couplings (smooth, single-valued and continuous) using	INR 57,84,480/-	No

			first principle based adiabatic to diabatic transformation (ADT). The procedure helps us to predict the feasibility (exothermicity and endothermicity) of a particular environmental reaction in a more accurate way.		
Calculation of Photoelectron Spectra of Cumulenes: Butatriene Molecule As a Test Example	MANIT, Bhopal	One year (2024-2025)	Application of BBO theory on Cumulenes systems and calculation of photoelectron spectra	INR 5,00,000/-	No

Publication							
Sl. No.	**Authors**	**Title**	**Journal**	**Vol. No. Page No.**	**Year**	**SCI/ Scopus**	**Impact Factor**
1.	Soumya Mukherjee, Bijit Mukherjee and Satrajit Adhikari	Five Electronic State Beyond Born–Oppenheimer Equations and Their Applications to Nitrate and Benzene Radical Cation	The Journal of Physical Chemistry A	121, 6314	2017	SCI	2.8
2.	Soumya Mukherjee, Bijit Mukherjee, Joy Dutta, Subhankar Sardar and Satrajit Adhikari	Topological Effects in Vibronically Coupled Degenerate Electronic States: A Case Study on Nitrate and Benzene Radical Cation	ACS Omega	3, 12465	2018	SCI	4.3
3.	Soumya Mukherjee, Joy Dutta, Bijit Mukherjee, Subhankar Sardar and Satrajit Adhikari	Conical Intersections and Nonadiabatic Coupling Terms in 1,3,5-$C_6H_3F_3^+$: A Six State Beyond Born-Oppenheimer Treatment	Journal of Chemical Physics	150, 064308	2019	SCI	3.1
4.	Soumya Mukherjee, Bijit Mukherjee, Subhankar Sardar and Satrajit Adhikari	Extended Born-Oppenheimer Equations for Non-Abelian Situations: A Study on NO_3 Radical and 1,3,5- $C_6H_3F_3^+$ Radical Cation	Computational and Theoretical Chemistry	1154, 57	2019	SCI	2.8
5.	Bijit Mukherjee,	Beyond Born-Oppenheimer Theory	International	38, 287	2019	SCI	3.1

	Koushik Naskar, Soumya Mukherjee, Sandip Ghosh, Tapas Sahoo and Satrajit Adhikari	for Spectroscopic and Scattering Processes	Reviews in Physical Chemistry				
6.	Koushik Naskar, Soumya Mukherjee, Bijit Mukherjee, Satyam Ravi, Saikat Mukherjee, Subhankar Sardar and Satrajit Adhikari	ADT: A Generalized Algorithm and Program for Beyond Born-Oppenheimer Equations of "N" Dimensional Sub-Hilbert Space	Journal of Chemical Theory and Computation	16, 1666	2020	SCI	5.5
7.	Joy Dutta, Soumya Mukherjee, Koushik Naskar, Sandip Ghosh, Bijit Mukherjee, Satyam Ravi and Satrajit Adhikari	The Role of Electron-Nuclear Coupling on Multi-State Photoelectron Spectra, Scattering Processes and Phase Transitions	Physical Chemistry Chemical Physics (Perspective)	22, 27496	2020	SCI	2.9
8.	Ankur Kumar Gupta, Vikash Dhindhwal, Michael Baer, Narayanasami Sathyamurthy, Satyam Ravi, Soumya Mukherjee, Bijit Mukherjee and Satrajit Adhikari	Non-Adiabatic Coupling and Conical Intersection(s) Between Potential Energy Surfaces for HeH_2^+	Molecular Physics	118, e1683243	2020	SCI	1.8
9.	Satyam Ravi, Soumya Mukherjee, Bijit Mukherjee, Satrajit Adhikari, Narayanasami Sathyamurthy and Michael Baer	Non-Adiabatic Coupling as a Frictional Force in the Formation of H_3^+ : a Model Dynamical Study	The European Physical Journal D	74, 1	2020	SCI	1.5
10.	Bijit Mukherjee, Koushik Naskar, Soumya Mukherjee, Satyam Ravi, K. R. Shamasundar,	Beyond Born-Oppenheimer Constructed Diabatic Potential Energy Surfaces for $F + H_2$ Reaction	The Journal of Chemical Physics	153, 174301	2020	SCI	3.1

	Debasis Mukhopadhyay and Satrajit Adhikari						
11.	Soumya Mukherjee, Satyam Ravi, Koushik Naskar, Subhankar Sardar and Satrajit Adhikari	A Beyond Born-Oppenheimer Treatment of $C_6H_6^+$ Radical Cation for Diabatic Surfaces: Photoelectron Spectra of its Neutral Analog Using Time-Dependent Discrete Variable Representation	The Journal of Chemical Physics	154, 094306	2021	SCI	3.1
12.	Satyam Ravi, Soumya Mukherjee, Bijit Mukherjee, Satrajit Adhikari, Narayanasami Sathyamurthy and Michael Baer	Non-Adiabatic Coupling as a Frictional Force in $(He, H, H)^+$ Dynamics and the Formation of HeH_2^+	Molecular Physics	119, e1811907	2021	SCI	1.8
13.	Soumya Mukherjee, Satyam Ravi, Joy Dutta, Subhankar Sardar and Satrajit Adhikari	Beyond Born-Oppenheimer based Diabatic Surfaces of 1,3,5-$C_6H_3F_3^+$ to Generate the Photoelectron Spectra using Time-Dependent Discrete Variable Representation Approach	Physical Chemistry Chemical Physics	24, 2185	2022	SCI	2.9
14.	Joy Dutta, Satyam Ravi, Soumya Mukherjee, Avik Kumar Ojha and Satrajit Adhikari	Jahn-Teller Effect in Orthorhombic Manganites : Ab Initio Hamiltonian and Roto-vibrational Spectrum	The Journal of Physical Chemistry A	126, 691	2022	SCI	2.8
15.	Soumya Mukherjee, Saikat Hazra, Sandip Ghosh, Saikat Mukherjee and Satrajit Adhikari	Trajectory Surface Hopping vs. Quantum Scattering Calculations on $D^+ + H_2$ and $H + H_2^+$ Reactions using Ab Initio Surfaces and Couplings	Chemical Physics	560, 111588	2022	SCI	2.0
16.	Saikat Hazra, Soumya Mukherjee, Satyam Ravi, Subhankar Sardar and Satrajit Adhikari	Construction of Beyond Born-Oppenheimer Based Diabatic Surfaces and Generation of Photoabsorption Spectra: The Touchstone Pyrazine ($C_4N_2H_4$)	ChemPhysChem	23, e202200482	2022	SCI	2.2
17.	Mantu Kumar Sah, Soumya Mukherjee, Koushik Naskar, Saikat Hazra and	Curl Condition: Existence of Sub-Hilbert Space for Molecular Species or Chemical Processes	International Journal of Quantum Chemistry	123, e27212	2023	SCI	2.0

	Satrajit Adhikari						
18.	Michael Baer, Soumya Mukherjee, Satyam Ravi, Satrajit Adhikari and Narayanasami Sathyamurthy	The Quantum Mechanical Non-adiabatic coupling Term as friction in the formation of DH_2^+	Advances in Quantum Chemistry	89, 291-304	2023	SCI	1.8
19.	Soumya Mukherjee, Koushik Naskar, Saikat Hazra, Mantu Kumar Sah and Satrajit Adhikari	Beyond Born-Oppenheimer Treatment for Multi-State Photoelectron Spectra, Phase Transitions of Solids and Scattering Processes	Journal of Physics: Conference Series	2769, 012012	2023	SCI	
20.	Mantu Kumar Sah, Soumya Mukherjee, Swagato Saha, Koushik Naskar and Satrajit Adhikari	Photoelectron Spectra of Benzene: Can Path Dependent Diabatic Surfaces Provide Unique Observables?	Journal of Chemical Physics	159, 244116	2023	SCI	3.1
21.	Koushik Naskar, Soumya Mukherjee, Sandip Ghosh and Satrajit Adhikari	Coupled 3D ($J \geq 0$) Time-Dependent Wave Packet Calculation for the F + H_2 Reaction on Accurate Ab Initio Multi-State Diabatic Potential Energy Surfaces	Journal of Physical Chemistry A	128, 1438	2024	SCI	2.8
22.	Soumya Mukherjee, Swagato Saha, Sandip Ghosh, Satrajit Adhikari, Narayanasami Sathyamurthy, Michael Baer	Quasi-classical Trajectory Calculations on a Two-state Potential Energy Surface Including Nonadiabatic Coupling Terms as Friction for D^+ + H_2 Collisions	Journal of Physical Chemistry A	128, 7691	2024	SCI	2.8
23.	Priyanka Trivedi, Soumya Mukherjee and Rampal Pandey	Synthetic Strategies and applications of Porous Framework Materials: Special Attention towards MOFs	SMS Bulletin	15, 43	2024		
24.	Mantu Kumar Sah, Soumya Mukherjee, Satyam Ravi and Satrajit Adhikari	Construction of first-principles-based adiabatic and diabatic Hamiltonians for the TiO_6^{8-} unit of the $BaTiO_3$ crystal: photoemission spectra and ferroelectricity	Physical Chemistry Chemical Physics	27, 15759	2025	SCI	2.9
25.	Saikat Hazra, Subhali Basu, Soumya Mukherjee, Satyam Ravi,	Construction of Beyond Born–Oppenheimer-Based Diabatic Surfaces of o-$C_6H_4F_2^+$ Radical Cation: Calculation of Photoelectron and Mass-Analyzed	ChemPhysChem	DOI: https://doi.org/10.1002/cphc.202500461	2025	SCI	2.2

	Subhankar Sardar and Satrajit Adhikari	Threshold Ionization Spectra					
26.	Radheshyam Trivedi, Amit Dubey and Soumya Mukherjee	Complex Beyond Born–Oppenheimer Theory: A New Perspective on the Jahn–Teller Distortion Phenomenon	Journal of Chemical Theory and Computation	21, 10166	2025	SCI	5.5
27.	Priyanka Kumari, Rampal Pandey and Soumya Mukherjee	Spin-Orbit Couplings vis-′a-vis Complex Beyond Born-Oppenheimer Theory for Non-Abelian Systems: F+H_2 as a Test Case	International Journal of Quantum Chemistry	under review	2025	SCI	2.0
28.	Mansi Sunil Parab, Akash Deep Das, Amit Dubey and Soumya Mukherjee	Trapping of Freon Gases on Silicon (100)-2 X 1 Surface: A Density Functional Theory Based Study	ChemistrySelect	under review	2025	SCI	2.0
29.	Kuldeep Nagar, Akash Deep Das, Amit Dubey and Soumya Mukherjee	The Role of Solvent Polarity on the Synthesis of Ibuprofen Molecule: A Density Functional Approach	International Journal of Chemical Kinetics	under review	2025	SCI	1.6

Event Organized/News		
Programme	**Duration**	**Coordinators**
National Workshop, "Interpretation of Instrumentation Methods in Sciences and Engineering (IIMSE-2025)"	24/03/2025-28/03/2025	Prof. Amit Dubey (Convener) Dr. Rampal Pandey (Coordinator) Dr. Harjinder Singh (Coordinator) Dr. Soumya Mukherjee (Coordinator)

Placements		
Project/PhD students registered for placement	**Average Package in INR**	**Status**
Kuldeep Nagar, M.Sc. Chemistry, 4th Sem student (Thesis Supervisor, Dr. Soumya Mukherjee)	37,000/- per month (Saatvik Solar Pvt Ltd. Ambala, Haryana)	Received offer after leaving MANIT, Bhopal

Citations			
	h-index	**i-10 index**	**Total Citations**
Google Scholar	13	13	377
Scopus	11		321

Outreach Activities		
Outreach Activities Name	Date	Details
Participant in "Current Trends In Green Chemistry" Webinar by Bhatter College, Dantan	Sep 16, 2024	Participated
Invited talk in "ACCW-2024" workshop (national)	Oct. 18, 2024	Delivered a lecture on "Theoretical Study of Potential Energy Surfaces & Applications of Gaussian Software" in VIT, Bhopal
Invited talk in PCAMC-2024 conference (international)	Dec. 14, 2024	Delivered a lecture on "Introduction of Complex Diabatization: Formulation and Applications" in IISERK, Kolkata
Invited talk in SRAPCR-2025 conference (international)	Apr. 10, 2025	Delivered a lecture on " Spin-Orbit Coupling vis-á-vis Complex Diabatization Approach: Formulation and Future Perspective" in IACS, Kolkata
Participant in "ISRO Academia Connect Workshop" in MANIT, Bhopal	May 22, 2025	Participated
One of the Doctoral Committee members		Invited as one of the Doctoral Committee members of Ms. Shalini Namdev, Ph.D scholar of Dr. Satyam Ravi, VIT, Bhopal
One of the Doctoral Committee members		Invited as one of the Doctoral Committee members of Ms. Kamini Vishwakarma, Ph.D scholar of Dr. Sumit Mittal, VIT, Bhopal

Other Contributions

(i) Departmental Positions:

- Website and Media Coordinator (dealing with Annual Report, Newsletter and Social Media Accounts)
- Post-Graduate Organic Chemistry Laboratory In-charge
- Member of Laboratory Equipment Purchase Committee
- Technical Committee member of the national workshop (short term training program), Advances in Material Research, Innovation and Technology (AMRIT-2025)

(ii) Institutional Positions:

- Technical Purchase Committee Member, Powder X-Ray Diffraction Spectrometer, Central Research Facility
- Committee Member for improving Publications, IPR & Patents, Externally Funded Projects, and Professional Practices for NIRF Ranking
- Faculty member for anti-ragging duty in Hostels 4, 10C and 10D from August, 2025-December, 2025.

(iii) Other Departmental and Institutional Level Responsibilities:

- ERP faculty advisor for B.Tech, first year (second semester), section A (January, 2024).
- One of the Book Fair coordinators in E-Summit'24 (February, 2024).
- One of the "Bhopal Darsan" coordinators for newly admitted B.Tech students (August, 2024 and

August, 2025).

- Duty of seating arrangement and discipline in Convocation, 2024 (December, 2024).
- One of the faculty coordinators in E-Summit'25 (February, 2025).
- One of the committee members of stock verification for hostel 10 (June, 2025).
- Actively involved in upgradation and modification of B.Tech Environmental Science (CHY 24110) and Engineering Chemistry Practical (CHY 24126) as well as several M.Sc. Physical Chemistry (CHY 24511, CHY 24521, CHY 24533 and CHY 24551) course contents.
- Introduced (with Dr. Sarvesh Kumar Pandey) one new elective Ph.D course work (CHY 24815) on "Advanced Quantum Chemistry and Applications" with credit point 3.