Curriculum vitae

Deb Pratim Mukhopadhyay

Assistant Professor

Department of Chemistry
School of Basic and Applied Sciences
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EDUCATION:

July 2011 - July 2018

Ph.D. in Physical Chemistry
Indian Association for The Cultivation of Science (IACS)
University of Calcutta, Kolkata, India

2009 - 2011

Master of Science (M. Sc.) in Chemistry
Indian Institute of Technology (IIT) Guwahati,
Guwahati, India
CPI: 8.93/10

2006 - 2009

Bachelor of Science (B. Sc.) in Chemistry
Presidency College, University of Calcutta, *Kolkata, India*
First Class (Honours)

WORK and RESEARCH EXPERIENCE:

March 2025- Present

Assistant professor at Adamas University
School of Basic and Applied Sciences
Department of Chemistry

September 2022 – August 2024

(2 years)

Postdoctoral researcher at **Synchrotron SOLEIL**
Saint-Aubin, France
Topic: *Photoelectron spectroscopy and study of Photoelectron Circular Dichroism (PECD) of biomolecules in gas phase using synchrotron radiation.*
Beamline: DESIRS
Advisor: Dr. Laurent Nahon

February 2021 – August 2022 (1 year 7 months)	**Postdoctoral researcher** at **J. Heyrovský Institute of Physical Chemistry**, Prague, Czech-Republic ***Topic:*** *Photodissociation of VOCs containing multiple halogen atoms using Velocity map imaging (VMI) technique.* **Department:** Dynamics of Molecules and Clusters **Advisor:** Dr. Michal Fárník
November 2018 – January 2021 (2 years 3 months)	**Postdoctoral researcher** at **University of Würzburg**, Würzburg, Germany ***Topic:*** *Study of photodissociation of reactive intermediates and VOCs using Velocity map imaging (VMI) technique.* *VUV Photoelectron spectroscopy of reactive intermediates (biradical, free radical, carbene) and study of reaction kinetics via coincidence spectroscopy (i²PEPICO) using synchrotron radiation.* **Advisor:** Prof. Dr. Ingo Fischer
July 2011 - July 2018	**Doctoral Research** at **Indian Association for the Cultivation of Science (IACS)**, Kolkata, India ***Thesis Title:*** *Laser Induced Fluorescence Spectroscopy and Excited State Dynamics of Hydrogen-Bonded Complexes of p-Fluorophenol Under Supersonic Jet Expansion.* **Supervisor:** Prof. Tapas Chakraborty
December – May 2011	**Master's thesis** at **Indian Institute of Technology (IIT) Guwahati**, Guwahati, India ***Dissertation Title:*** *Solvatochromic study of alkylated product of 2-(4'-N, N-dimethylaminophenyl) pyrido [3, 4-d] imidazole.* **Supervisor:** Dr. G. Krishnamoorthy
May – July 2010	**Summer research project** at **Indian Association for the Cultivation of Science (IACS)**, Kolkata, India ***Project Title:*** *Study on excited-state double proton transfer (ESDPT) of 7-Azaindole with cyclic amide.* **Supervisor:** Prof. Tapas Chakraborty

RESEARCH INTERESTS:

Gas-phase spectroscopy is the only method capable of uncovering the intrinsic properties of solvent-free, isolated systems, ranging from atoms to biomolecules, aerosols to clusters, and free radicals to organometallics, with a unique level of detail. My research career takes a bottom-up approach to understanding chemical complexities by investigating these detailed aspects of bonding, reactivity, and photoinduced processes of cold, isolated molecules, free radicals, reactive intermediates, and molecular clusters in the gas phase. Using various advanced spectroscopic techniques aided with quantum chemical calculations, I aim to address some of the fundamental questions of chemical dynamics and light-matter interactions.

♦ Photoelectron circular dichroism (PECD) of biomolecules:

My current research is centered on photoelectron spectroscopy and the study of biomolecular homochirality, such as ribose sugar, amino acids, and dipeptides, in the gas phase. The main challenge of this research is efficiently vaporizing these extremely low volatile, thermolabile molecules and to achieve that I am using an advanced vaporization technique involving aerosol thermo-desorption. By utilizing narrowband, tunable, circularly polarized synchrotron light between 8 to 14 eV with double imaging photoelectron-photoion coincidence spectroscopy (i^2PEPICO), I able to measure the photoelectron spectra and study the photoelectron circular dichroism (PECD) of these chiral biomolecules to explore their intrinsic chirality and the origins of homochirality in nature. This study also provides valuable insights into the nature of electronic states and fragmentation patterns associated with radiation damage. ***(Ongoing)***

♦ State selective photodissociation with 2-Dimensional Photofragment Imaging :

I have studied the state selective photodissociation of key atmospheric free radical and halogenated VOCs using 2-dimensional photofragment velocity map imaging (VMI). Transient intermediates were generated by pyrolyzing suitable precursors in the gas phase with a Silicon carbide (SiC) microreactor. Through the pump-probe method, I investigated the mechanistic details and dissociation dynamics from various electronic states. In this context, I have developed a new, efficient VUV scheme for detecting fragmented Cl which in general detected by (2+1) or (3+1) UV-REMPI. Our new approach avoids unwanted multiphoton side reactions and improves photoionization efficiency due to single-photon absorption process. ***(3 Publications)***

♦ Photoelectron-Photoion Coincidence Spectroscopy of Reactive Intermediates:

Transient, highly reactive intermediates (biradicals, free radicals, carbenes) formed during reactions often dictate the outcome of complex multistep reactions and the catalytic efficiency of main group compounds. My research has focused on various inorganic and organic intermediates, such as BH, BH_2, P=CH_2, P-CH_3, and Bi-CH_3, isolable only in the gas phase. Using photoelectron-photoion coincidence spectroscopy (i^2PEPICO) and VUV synchrotron radiation (6-18 eV), I measured mass-selected photoelectron spectra (ms-PES) to explore their bonding, dissociative photoionization thresholds, cationic structures, energetics, and conformational landscapes. I reported the first experimentally measured value of singlet-triplet band gap for BH and revised the Bi-C single bond energy, vital for Bi-based catalysts. This study helps to understand the underlying chemistry, reactivity, the nature of electronic states and fragmentation patterns of cations of these transient species. Additionally, I investigated the reaction kinetics of organic radicals with O_2 in an isomer-selective manner. Radicals were generated by photolysis, with concentrations measured by probing specific PES bands. The photolysis pulse defined T0, and the kinetic trace was measured continuously using synchrotron light and PEPICO. ***(6 Publications)***

♦ Laser Induced Fluorescence (LIF) Spectroscopy of H-Bonded Clusters:

During my Ph.D. research, I investigated the structural and photophysical behavior of hydrogen-bonded binary complexes of p-fluorophenol under supersonic jet expansion using laser-induced fluorescence (LIF) spectroscopy. The goal was to understand how a single solvent molecule can alter the photophysical properties of the phenolic moiety near the bottom of the S_1 potential energy well. By measuring fluorescence excitation and dispersed fluorescence spectra (single vibronic level fluorescence), I studied excited state phenomena such as Fermi interaction, mode mixing, and energy-dependent vibrational energy relaxation (IVR). These phenomena were examined by systematically introducing excess vibronic energy into the clusters. Our study revealed the details of how energy threshold and nature of IVR and inter-mode couplings change due to hydrogen bonding with a single solvent molecule (H_2O, CH_3OH, THF), providing insights into the photo-induced processes of solvated phenolic groups. ***(3 Publications)***

- **Fluorescence Spectroscopy in Gas Phase and Cryogenic Condition:**

Various fluorophenols are studied in the gas phase and cold inert solvents by steady-state absorption and fluorescence spectroscopy for a better understanding of the origin of the perfluoro effect. We have explored the alteration of photophysical processes of these compounds, due to the lowering of dark πσ* states after the gradual introduction of fluorine atoms at different positions of the phenolic ring. ***(1 Publication)***

- **Matrix Isolated IR Spectroscopy:**

Infrared spectroscopy of binary complexes of fluorophenols isolated in cold (~8K) inert gas matrix is investigated for a better understanding of the correspondence between the observed spectral shifts with theoretically predicted intermolecular interactions. ***(1 Publication)***

PUBLICATIONS:

1. J. Janoš, I. S. Vinklárek, J. Rakovský, **D. P. Mukhopadhyay**, B. F. E. Curchod, M. Fárník* and P. Slavíček*, On the Wavelength-Dependent Photochemistry of the Atmospheric Molecule CF_3COCl, ***ACS Earth Space Chem***., 7, 2275 (2023) DOI:10.1021/acsearthspacechem.3c00196

2. D. Schleier, M. Gerlach, D. Schaffner, **D. P. Mukhopadhyay**, P. Hemberger* and I. Fischer*, Threshold photoelectron spectroscopy of trimethylborane and its pyrolysis products, ***Phys. Chem. Chem. Phys.,*** 25, 4511 (2023) DOI: 10.1039/D2CP04513C

3. D. Schleier, M. Gerlach, **D. P. Mukhopadhyay**, E. Karaev, D. Schaffner, P. Hemberger* and I. Fischer*, Ammonia borane, NH_3BH_3 – A threshold photoelectron-photoion coincidence study of a potential hydrogen storage material, ***Chem. Eur. J.,*** 28, e202201378 (2022) [Cover Feature] DOI: 10.1002/chem.202201378

4. **D. P. Mukhopadhyay*,** M. Gerlach, S. Hartweg, I. Fischer* and J. C. Loison, Photoelectron spectroscopy of low valent organophosphorus compounds, P-CH_3, H-P=CH_2 and P=CH_2, ***Phys. Chem. Chem. Phys.,*** 24, 10993 (2022) DOI: 10.1039/d2cp01082h

5. C. T. Matthaei, **D. P Mukhopadhyay**, A. Röder, L. Poisson, I. Fischer*, Photodissociation of the trichloromethyl radical: photofragment imaging and femtosecond photoelectron spectroscopy. ***Phys. Chem. Chem. Phys.,*** 24, 928 (2022) DOI: 10.1039/d1cp04084g

6. C. T. Matthaei, **D. P. Mukhopadhyay***, and I. Fischer*, Photodissociation of Benzoyl Chloride: A Velocity Map Imaging Study Using VUV Detection of Chlorine Atoms. ***J. Phys. Chem. A,*** 125, 2816 (2021) DOI: 10.1021/acs.jpca.0c11236

7. D. Schleier, E Reusch, M. Gerlach, T. Preitschopf, **D. P. Mukhopadhyay**, N. Faßheber, G. Friedrichs*, P. Hemberger* and I. Fischer*, Kinetics of 1- and 2-methylallyl + O_2 reaction, investigated by photoionisation using synchrotron radiation. ***Phys. Chem. Chem. Phys.***, 23, 1539 (2021) DOI: 10.1039/d0cp05441k

8. **D. P. Mukhopadhyay**, D. Schleier, S. Wirsing, J. Ramler, D. Kaiser, E. Reusch, P. Hemberger, T. Preitschopf, I. Krummenacher, B. Engels*, I. Fischer* and C. Lichtenberg*, Methylbismuth: an organometallic bismuthinidene biradical. ***Chem. Sci.***, 11, 7562 (2020) [2020 Chemical Science HOT Article and front cover] DOI: 10.1039/d0sc02410d

9. **D. P. Mukhopadhyay**, D. Schleier, I. Fischer*, J. C. Loison, C. Alcaraz, and G. A. Garcia, Photoelectron spectroscopy of boron-containing reactive intermediates using synchrotron radiation: BH_2, BH, and BF. ***Phys. Chem. Chem. Phys.***, 22, 1027 (2020) [2019 PCCP HOT Article and editor's choice] DOI: 10.1039/c9cp06010c

10. **D. P. Mukhopadhyay**, S. Biswas, A. Chattopadhyay, T. Chakraborty*, Conformational Preference Determined by C-H···π Interaction of an O-H···O Hydrogen Bonded Binary Complex of p-Fluorophenol with 2,5-Dihydrofuran: A Laser-Induced Fluorescence Spectroscopy Study. ***J. Phys. Chem. A,*** 122, 3787 (2018) DOI: 10.1021/acs.jpca.8b01384

11. **D. P. Mukhopadhyay**, S. Biswas, T. Chakraborty*, Intermolecular vibrations and vibrational dynamics of a phenol···methanol binary complex studied by LIF spectroscopy. ***Chem. Phys. Lett.,*** 674, 71 (2017) DOI: 10.1016/j.cplett.2017.02.059

12. **D. P. Mukhopadhyay**, S. Biswas, T. Chakraborty*, LIF spectroscopy of *p*-fluorophenol···water complex: Hydrogen bond vibrations, Fermi resonance and vibrational relaxation in the excited state. ***J. Phys. Chem. A,*** 120, 9159 (2016) DOI: 10.1021/acs.jpca.6b08988

13. P. Banerjee, **D. P. Mukhopadhyay**, T. Chakraborty*, On the Origin of Donor O–H Bond Weakening in Phenol-Water Complexes. ***J. Chem. Phys.,*** 143, 204306 (2015) DOI: 10.1063/1.4936208

14. S. Karmakar, **D. P Mukhopadhyay**, T. Chakraborty*, Electronic spectra, and excited-state dynamics of pentafluoro phenol: Effects of low lying $\pi\sigma^*$ states. ***J. Chem. Phys.,*** 142, 184303 (2015) DOI: 10.1063/1.4919950

IDENTIFIERS:

- Scopus id: 56640760700
- Researcher id (Web of Science): AAG-7935-2019
- ORCID id: 0000-0002-2759-1934
- Google scholar link: https://scholar.google.com/citations?hl=en&user=ndRdbi4AAAAJ

EXPERTISE IN VARIOUS TECHNIQUES:

- 2D Velocity map imaging (VMI) technique with pump-probe experimental set-up coupled with linear TOF mass spectrometer.
- Pyrolysis and flash photolysis for generating reactive species in the gas phase and hands-on experience in their reaction kinetics study.
- Experience of working with double imaging PEPICO spectrometer using VUV beamlines in synchrotron facilities (Swiss light source and SOLEIL, France).
- Designing and fabrication of laser induced fluorescence (LIF) experimental set-up coupled with supersonic jet expansion and tunable UV laser. Both fluorescence excitation and dispersed fluorescence spectra can be measured simultaneously by this instrument.
- Building of an instrumental set up for doing UV absorption and fluorescence spectroscopic studies of matrix isolated cold molecules (~ 8K).
- Working experience in home-built low temperature (up to 130K) fluorescence spectroscopy set up. Temperature can be varied using cold nitrogen vapor and the fluorescence signal is collected by a commercial fluorometer.

- Developed a Raman spectrometer using a 532 nm continuous diode laser.
- Practical experience in high vacuum systems (10^{-8} mbar).
- Working experience in developing a long path absorption photometer (LOPAP) for in situ measurement of atmospheric HONO.
- Working with HPLC system with super critical CO_2.
- Computational package handled: Gaussian 09, GAMESS (USA), PGOPHER.
- Programming and interfacing in LABVIEW
- Instruments handled:

  - TOF mass spectrometer
  - Pulsed Nd-YAG lasers, Dye lasers, Diode laser
  - Xenon arc lamp (Newport) and Deuterium lamp (Hamamatsu)
  - FTIR spectrometer (Bruker Tensor 27)
  - UV-Vis spectrometer (Schimadju, Perkin-Elmer)
  - Fluorometer (Fluoromax- 3,4; Fluorolog 3)
  - CCD (Synapse, Horiba), PMT, MCP, DLD
  - Monochromator (iHR 550, Horiba)

TEACHING EXPERIENCES:

- Theory Course:
  - Statistical Mechanics (M. Sc, Chemistry)
  - Analytical Techniques (B. Sc, Microbiology & Biochemistry)
  - Organo-Physical Chemistry (B. Sc, Biotechnology)
  - Applied Science (B. Tech, Engineering)

- Laboratory Course:
  - Organo-Physical Chemistry Laboratory (B. Sc, Biotechnology)

- I have supervised one experiment (Franck-Hertz experiment) in the bachelor lab course of physical chemistry in the University of Würzburg, Germany during summer and winter semesters of 2019-2020. It includes both supervision and evaluation of students of chemistry, biochemistry, science education and material science. In this experiment, students are expected to use basic concepts of quantum mechanics to interpret the experimental observations.

OTHER EXPERIENCES:

- Worked as a reviewer in *Phys. Chem. Chem. Phys.* (RSC) journal.
- Worked as Cultural Secretary of hostel "Siang" at IIT Guwahati (2010-2011).

AWARDS AND FELLOWSHIPS:

- **Best poster award**, 739 Wilhelm Und Else Heraeus Seminar on Molecular Physics and Physical Chemistry with Advanced Photon Sources, 2022, Germany
- International Travel Support **(ITS),** Science and Engineering Research Board (SERB), DST
- Graduate Aptitude Test for Engineering **(GATE-2011)** in Chemical Science (All India rank-233)
- Fellowship for doctoral research through National Eligibility Test **(NET-2010)** (All India rank-115)
- Selected through Joint Admission test for Masters **(JAM- 2009)**

SCIENTIFIC CONFERENCES:

- 24th European Conference on the Dynamics of Molecular Systems (MOLEC-2024), Aarhus, Denmark, 2024 (**Poster presentation**)
- 13th Conference on Isolated Biomolecules and Biomolecular Interactions (IBBI-2024), Hamburg, Germany, 2024 (**Oral Presentation**)
- 11th International Meeting on Atomic and Molecular Physics and Chemistry (IMAMPC-2022), 2022, Prague, Czech Republic (**Poster presentation**)
- 739 Wilhelm Und Else Heraeus Seminar on Molecular Physics and Physical Chemistry with Advanced Photon Sources, 2022, Germany (**Best Poster award**)
- Bunsentagung (120 th General Assembly of the German Bunsen Society for Physical Chemistry), Germany, 2021 (**Oral presentation**)
- Bunsentagung (118 th General Assembly of the German Bunsen Society for Physical Chemistry), Germany, 2019
- Structure and Dynamics of Molecules and Clusters (SDMC-2016), India (**Poster presentation**)
- Trombay Symposium on Radiation and Photochemistry (TSRP-2014), India (**Poster presentation**)
- National Symposium on Non-Equilibrium Statistical Physics and Nonlinear Dynamics, India 2014
- National Symposium on Radiation and Photochemistry (NSRP-2013), India (**Poster presentation**)
- An International Conference on Electronic Structure and Dynamics of Molecules and Clusters, India, 2013
- International Symposium on Chemistry and Complexity, India, 2011

INVITED TALKS:

- State selective photodissociation of chlorine-containing volatile organic compounds (VOCs) and free radicals in isolated condition, Meeting on the "Fundamental processes in Isolated Systems", SOLEIL, France, 2024
- Photodissociation of chlorine containing volatile organic compounds (VOCs) and free radicals in isolated condition: A 2D Photofragment imaging study, "12th Future of Chemistry- Symposium series", TIFR, India, 2023

- Low frequency vibrations, vibrational dynamics and energetics of Hydrogen-bonded binary clusters of fluorophenol under isolated condition, University of Würzburg, Germany, 2018

Detailed Academic Qualifications:

Year of passing	Level	Board/University	Subjects	Marks (%/CPI)
2011	M. Sc.	IIT Guwahati	Chemistry	8.93/10.0
2009	B. Sc.	Calcutta University	Chemistry (Hons), Physics, Mathematics	67.0 %
2006	Higher Secondary	W.B.C.H.S.E (State board)	Physics, Chemistry, Mathematics, Biology	81.8 %
2004	Secondary	W.B.B.S.E (State board)	Bengali, English, Math, Physical Science, Life science, History, Geography	80 %

Personal Information:

- Date of birth: 15-July-1989
- Place of birth: West Bengal, India
- Nationality: Indian