



SAPTARSI MONDAL

Postdoctoral researcher
Department of Chemistry,
University of Texas at Austin, USA

Nationality

Sex



India

Male

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<https://scholar.google.com/citations?user=nIOXRPcAAAAJ&hl=en>

SUMMARY



Ultrafast and multidimensional IR spectroscopy expert with 12+ years of experience in vibrational dynamics, polariton chemistry, plasmonic materials, and electrochemical interfaces. Published 26+ peer-reviewed articles, including front-cover papers and invited reviews, and developed new analytical methods such as wavelet-based denoising for ultrafast spectroscopy.

WORK EXPERIENCE



Postdoctoral Researcher

Department of Chemistry, University of Texas at Austin (QS ranking: 65)

Nov 2024 - Present (1 year 6 months +) **Advisor: Prof. Carlos R. Baiz**

- Hydrogen bond dynamics of water at plasmonic electrode surface by 2D-IR spectroscopy.
- Polariton/plasmonic nanocrystals for altering chemical reactions and energy applications



Postdoctoral Researcher

Department of Chemistry, University of Michigan (QS ranking: 32)

Nov 2023 - Nov 2024 (1 year) **Advisor: Prof. Kevin J. Kubarych**

- Environmentally and biologically relevant enzyme catalysis reactions using vibrational light-matter strong coupling inside an optical cavity (Polariton Chemistry) using 2D-IR spectroscopy.



Research Professor

IBS-CMSD, Korea University (QS ranking: ~79)

Mar 2019 – Aug 2023 (4 years 6 months) **Advisor: Prof. Minhaeng Cho**

- Discrete wavelet transform based denoising for enhanced S/N for ultrafast spectroscopy.
- Water structure and dynamics in the biocompatible polymer and hydrogel.
- Free volume element (FVE) size and probability distribution in acrylate-based biocompatible polymer.
- Ion transport mechanism in Li-ion battery.



Visiting Researcher

Molecular Spectroscopy Laboratory, RIKEN

Aug 2018 – Sep 2018 (2 months) **Advisor: Prof. Tahei Tahara**

- DNA Induced Reorganization of Water at Lipid membrane Interfaces using heterodyne detected vibrational sum frequency generation spectroscopy

EDUCATION



Indian Association for the Cultivation of Science

Ph.D., Chemistry (University of Calcutta)

2013 - 2018

Thesis Advisor Prof. Prashant Chandra Singh

Thesis Title Role of Weak Noncovalent Interactions in the Solvation and Photophysical Properties of Atmospherically and Biologically Relevant Molecules



IIT Bombay

Master of Science, Physical Chemistry

2011 – 2013

CGPA 8.44



Ramakrishna Mission Vidyamandira

Bachelor of Science (Hons.), Chemistry

2008 – 2011

67.13%

RESEARCH INTEREST



Technique

- Two-dimensional infrared (2D IR) spectroscopy
- Ultrafast vibrational transient grating spectroscopy
- Polarization-selective mid-infrared pump-probe (IR PP) spectroscopy

System

- Biocompatible polymer thin film and hydrogel
- 'Water in Li-salt' electrolyte for Li-ion battery application, separator membrane for Li-ion battery
- Vibrational polariton
- Plasmonic nanocrystal
- Interfacial electrochemistry e.g. hydrogen evolution (HER), and CO₂ reduction reaction (CO₂RR)
- Protein and DNA in deep eutectic solvent
- Intrinsically disordered protein, misfolded proteins (Amyloids).
- Biological membrane and DNA-lipid interaction

LIST OF PUBLICATION

Book Chapter

1. Mondal, S., Lee, E., Baiz, C.R. (2026). Dimethyl Sulfoxide (DMSO) Interactions with Water, Organic Solvents, and Biomolecules: A Molecular Perspective. In: Langley, N., Almarsson, Ö., Osborne, D.W. (eds) The Pharmaceutical Applications of Dimethyl Sulfoxide. AAPS Advances in the Pharmaceutical Sciences Series, vol 30. Springer, Cham. https://doi.org/10.1007/978-3-032-19256-1_2

Manuscript under preparation

1. Mondal S.; Kwak* K.; Cho* M. Electrolyte Swelling Dynamics on Polymer Separator Membrane Revealed by ATR-FTIR, 2D-correlation Spectroscopy and Quantum Chemical Calculations.
2. Mondal S.; Park K; Palchowdhury S.; Kwak* K.; Cho* M. Battery Separators as Active Regulators of Ion Solvation and Transport.

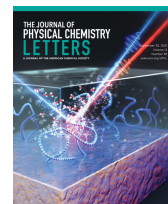
Manuscript under revision

1. Mondal S., Chen K., Baiz* C. Cosolvents Disrupt Water H-bond Networks at Electrode Interfaces: a Surface-enhanced 2D IR Study *ChemRxiv* **2025**; doi:10.26434/chemrxiv-2025-4jhpj (*JACS*)
2. Mondal S.; Jeon J.; Cho M., Baiz* C. Two-Dimensional Infrared Spectroscopy in Complex Environments *Chem. Rev.* **2026**

Published

1. Starkey C., Mondal S., Baiz* C. Machine Learning Potentials Accurately Reproduce Vibrational Dynamics in Complex Environments *J. Chem. Phys.* **2025**, 163, 234116
2. Mondal, S.; Al-Mualem, Z.; Cardenas, A. E.; Hazarika, S.; Ren, H.; Baiz, C. R.* Tuning Hydrogen Bond Networks at Gold Electrodes: A Study of Potential-Dependent DMSO-Water Interfaces *ACS Electrochem.* **2025**, 1(5), 709-716.
3. Palchowdhury S.; Mondal S.; Kwak K., Cho M.* Recasting the wobbling-in-a-cone model for the rotational anisotropy of phenylselenocyanate in poly(methyl methacrylate): Effect of internal bond rotation and polymer segmental motion. *J. Chem. Phys.* **2024**, 161, 214112.

4. Chakraborty D.; Chatterjee R.; Mondal S.; Das S. K.; Cho M., Bhaumik A.* Construction of N-rich Amino-Linked Porous Organic Polymers for Outstanding Precombustion CO₂ capture and H₂ Purification: A Combined Experimental and Theoretical Study. *ACS Appl. Mater. Interfaces* **2023**, 15, 41, 48326-48335.
5. Mondal*, S. Charge-shifted Weak Noncovalent Interactions in the Atmospherically Important OCS Microhydrated Complexes: A Computational and Topological Perspective. *J. Phys. Chem. A* **2023**, 127, 15, 3293-3304 (selected as the front cover).
6. Boruah, T.; Das, S. K.; Kumar, G.; Mondal, S.; Dey*, R. S. Dual active sites in a triazine-based covalent organic polymeric framework promoting oxygen reduction reaction, *Chem. Commun.* **2022**, 58, 5506-5509.
7. Mondal, S.; Kang, J.; Park, K.; Lim J. M.; Ha J.-H.; Kwak, K.; Cho, M. Adsorbed Water Structure on Acrylate-based Biocompatible Surface, *J. Phys. Chem. Lett.* **2021**, 12, 9275-9282 (Selected as the journal cover)
8. Chowdhury, A.; Das, S. K.; Mondal, S.; Ruidas, S.; Chakraborty, D.; Chatterjee, S.; Bhunia, M. K.; Chandra, D.; Hara, M.; Bhaumik, A. Sulfur-containing nitrogen-rich robust hierarchically porous organic polymer for adsorptive removal of mercury: experimental and theoretical insights. *Environ. Sci.: Nano* **2021**, 8, 2641-2649
9. Sahu, P.; Kim, J.; Park, K.; Kim, E.; Mondal, S.; Kwak, K.; Cho, M. Solvation structure of phosphonium ionic liquid/CH₃SCN mixture as electrolytes for Li-ion batteries: Infrared pump-probe spectroscopic studies. *Bull. Korean Chem. Soc.* **2021**, 43(2), 215-221.
10. Das, S. K.; Shyamal, S.; Das, M.; Mondal, S.; Chowdhury, A.; Chakraborty, D.; Dey, R. S.; Bhaumik, A. Metal-free Pyrene-based Conjugated Microporous Polymer Catalyst Bearing N and S-sites for Photo-Electrochemical Oxygen Evolution Reaction. *Front. Chem.* **2021**, 9, 1094
11. Park, J. Y.#; Mondal, S.#; Kwon, H.J.; Han, H.; Kwak, K.; Cho, M. Effect of Isotope Substitution on the Fermi Resonance and Vibrational Lifetime of Unnatural Amino Acids Modified with IR probe: A 2D-IR and Pump-probe Study of 4-Azido-L-Phenyl Alanine. *J. Chem. Phys.* **2020**, 153 (16), 164309 [Equal contribution]
12. Nandy, T.; Mondal, S.; Singh P.C. Fluorine induced conformational switching and modulation in photophysical properties of 7-fluorotryptophan: Spectroscopic, quantum chemical calculation and molecular dynamics simulation studies, *J. Photochem. Photobiol.* **2020**, 3, 100011
13. Park, J. Y.#; Kwon, H.J.#; Mondal, S.; Han, H.; Kwak, K.; Cho, M. Two-dimensional IR spectroscopy reveals a hidden Fermi resonance band in the azido stretch spectrum of β -azidoalanine. *Phys. Chem. Chem. Phys.* **2020**, 22 (34), 19223-19229. [Equal contribution]
14. Das, S.; Chatterjee, S.; Mondal, S.; Modak, A.; Chandra, B. K.; Das, S.; Nessim, G. D.; Majee, A.; Bhaumik, A. Thiadiazole containing N- and S-rich highly ordered periodic mesoporous organosilica for efficient removal of Hg(II) from polluted water. *ChemComm.* **2020**, 56 (28), 3963-3966.
15. Nandy, T.; Mondal, S.; Singh, P. C. Solvent organization around the noncanonical part of tyrosine modulates its fluorescence properties. *Phys. Chem. Chem. Phys.* **2019**, 21, 6042-6050
16. Mondal, S.; Chatterjee, S.; Mondal, S.; Bhaumik, A. Thioether-Functionalized Covalent Triazine Nanospheres: A Robust Adsorbent for Mercury Removal. *ACS Sustain. Chem. Eng.* **2019**, 7 (7), 7353-7361.
17. Mondal, S.; Biswas, B.; Nandy, T.; Singh, P. C. Understanding the Role of Hydrophobic Terminal in the Hydrogen Bond Network of the Aqueous Mixture of 2,2,2-Trifluoroethanol: IR, Molecular Dynamics, Quantum Chemical as Well as Atoms in Molecules Studies. *J. Phys. Chem. B* **2018**, 122 (25), 6616-6626.
18. Das, S. K.; Bhanja, P.; Kundu, S. K.; Mondal, S.; Bhaumik, A. Role of Surface Phenolic-OH Groups in N-Rich Porous Organic Polymers for Enhancing the CO₂ Uptake and CO₂/N₂ Selectivity: Experimental and Computational Studies. *ACS Appl. Mater. Interfaces* **2018**, 10 (28), 23813-23824.
19. Mondal, S.; Chatterjee, S.; Halder, R.; Jana, B.; Singh, P. C. Role of Dispersive Fluorous Interaction in the Solvation Dynamics of the Perfluoro Group Containing Molecules. *J. Phys. Chem. B* **2017**, 121 (32), 7681-7688.



20. Mondal, S.; Biswas, B.; Sarkar, S.; Singh, P. C. A combined molecular dynamics simulation, atoms in molecule analysis and IR study on the biologically important bulk fluorinated ethanols to understand the role of weak interactions in their cluster formation and hydrogen bond network. *J. Mol. Liq.* **2017**, 240 (Supplement C), 708-716.
21. Mondal, S.; Biswas, B.; Nandy, T.; Singh, P. C. Hydrophobic fluorine mediated switching of the hydrogen bonding site as well as orientation of water molecules in the aqueous mixture of monofluoroethanol: IR, molecular dynamics and quantum chemical studies. *Phys. Chem. Chem. Phys.* **2017**, 19 (36), 24667-24677.
22. Biswas, B.; Mondal, S.; Singh, P. C. Combined Molecular Dynamics, Atoms in Molecules, and IR Studies of the Bulk Monofluoroethanol and Bulk Ethanol to Understand the Role of Organic Fluorine in the Hydrogen Bond Network. *J. Phys. Chem. A* **2017**, 121 (6), 1250-1260.
23. Mondal, S.; Halder, R.; Biswas, B.; Jana, B.; Singh, P. C. Solvent organization around the perfluoro group of coumarin 153 governs its photophysical properties: An experimental and simulation study of coumarin dyes in ethanol as well as fluorinated ethanol solvents. *J. Chem. Phys.* **2016**, 144 (18), 184504.
24. Biswas, B.; Mondal, S.; Singh, P. C. Role of Hydrogen Bond in the Solvation Behavior of the Binary Mixtures Containing Fluorocarbon Alcohol Molecules and Chloroform: An Experimental and Theoretical Study. *ChemistrySelect* **2016**, 1 (18), 5607-5617 [Equal contribution]
25. Mondal, S.; Teja, A. U.; Singh, P. C. Effect of microhydration on the atmospherically important metastable carbonyl sulfide anion: Structure, energetic, and infrared study. *Int. J. Quantum Chem.* **2015**, 115 (12), 785-795.
26. Mondal, S.; Teja, A. U.; Singh, P. C. Theoretical Study on the Microhydration of Atmospherically Important Carbonyl Sulfide in Its Neutral and Anionic Forms: Bridging the Gap between the Bulk and Finite Size Microhydrated Cluster. *J. Phys. Chem. A* **2015**, 119 (15), 3644-3652.
27. Mondal, S.; Singh, P.C. Noble gas induced surprisingly higher stability of [small pi] hydrogen bonded complex: comparative study of hydrogen bonded complexes of HKrCCH and HCCH with H₂O, NH₃, CH₃OH and CH₃NH₂. *RSC Advances* **2014**, 4 (40), 20752-20760.

PROFICIENCY AND SKILLS



- Two-dimensional infrared (2D IR) spectroscopy
- Ultrafast vibrational transient-grating spectroscopy
- Polarization selective mid-infrared pump-probe (IR-PP) spectroscopy
- Ultrafast fluorescence upconversion spectroscopy
- Time-correlated single-photon counting (TCSPC)
- FT-IR, Raman spectroscopy and microscopy, Steady-state UV-Vis and Fluorescence spectroscopy, Dynamic light scattering, and NMR spectroscopy
- Ab-initio quantum chemistry, DFT calculation, GROMACS MD simulation, Atoms in Molecules (AIM)
- MATLAB, OriginPro, Adobe creative cloud suites including Photoshop, Illustrator, Lightroom.

SCHOLASTIC ACHIEVEMENTS



- Best poster award in Photochemistry in the 14th International DAE-BRNS Biennial Conference on Radiation & Photochemistry, January 2018
- Qualified Graduate Aptitude Test in Engineering (GATE-2013)
- Ranked in CSIR UGC NET examination: UGC-74 (Dec 2012), UGC- 81 (June 2013).
- Ranked 73 in Joint Admission Test for M.Sc. in IITs (JAM) in 2011.
- INSPIRE Scholarship by Government of India for excellent performance in 12th Level Examination.

CONFERENCES AND SEMINARS



- Oral presentation in the 78th International Symposium on Molecular Spectroscopy at University of Illinois at Urbana-Champaign (2025)
- Poster presentation in the 129th general meeting of Korean Chemical Society (2022)

- Invited talk in the Electronic Structure, Dynamics and Spectroscopy conference in IACS (2018)
- Poster in the 14th DAE-BRNS conference on Radiation & Photochemistry at BARC, Mumbai (2018)
- Invited talk in the departmental seminar (Physical Chemistry and Spectroscopy) at IACS (2018)
- Poster on in the 20th CRSI National Symposium in Chemistry at Gauhati University, Guwahati (2017)
- Invited talk in the departmental seminar (Physical Chemistry and Spectroscopy) at IACS (2017).
- National seminar “Frontier Areas of Chemistry-A Modern Perspective” at RKMV, Belur Math (2010).
- National Workshop on “The Origin of Modern Chemistry” at Scottish Church College, Kolkata (2010).

REFeree



- Prof. Minhaeng Cho | IBS-CMSD | Korea University, Seoul | ✉ mcho@korea.ac.kr
- Prof. Carlos Baiz | Department of Chemistry | University of Texas at Austin | ✉ cbaiz@cm.utexas.edu
- Prof. Kevin Kubarych | Department of Chemistry | University of Michigan | ✉ kubarych@umich.edu
- Prof. Kyungwon Kwak | IBS-CMSD | Korea University, Seoul | ✉ kkwak@korea.ac.kr
- Prof. Prashant Chandra Singh | School of Chemical Sciences | IACS, Kolkata | ✉ sppcs@iacs.res.in