

## Piyush Mishra

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### Education & Research Experience:

May 2024-Present	Assistant Professor (Grade-I)	Department of Chemistry Indian Institute of Technology, Kharagpur
Dec 2023-May 2024	Assistant Professor (Grade-I)	Department of Chemistry and Chemical Biology Indian Institute of Technology (Indian School of Mines), Dhanbad
Nov 2022-Present	MIT Affiliate Prof. Robert W. Field Prof. Brett A. McGuire	Department of Chemistry Massachusetts Institute of Technology, MA, USA
Apr 2023-October 2023	Postdoctoral Fellow Postdoc Advisor Prof. Albert Stolow	Advanced Research Complex University of Ottawa, ON, Canada
Dec 2019 - Nov 2022	Postdoctoral Associate Postdoc Advisor Prof. Robert W. Field	Department of Chemistry Massachusetts Institute of Technology, MA, USA
Aug 2015 - Nov 2019	Ph.D. Ph.D. Advisor Prof. Timothy S. Zwier (GPA: 4/4)	Department of Chemistry Purdue University, West Lafayette, IN, USA
Aug 2010 - May 2015	BS-MS Dual Degree Thesis Supervisor Prof. K.S.Viswanathan (CPI: 8.5/10)	Chemistry Major Indian Institute of Science Education and Research- Mohali, PB, India

### Awards and Recognition:

- 1) 39<sup>th</sup> rank in the 10<sup>th</sup> Junior Mathematics Olympiad (JMO) Kendriya Vidyalaya Sangathan system (2007-2008).
- 2) KVPY (Kishore Vaigyanik Protsahan Yojana) fellow (A Government of India Fellowship to encourage young scientists). Received scholarship from Class XII through BS-MS dual degree in science (2008).
- 3) Member of the Chemistry Honorary Society: Phi Lambda Upsilon (PLU)- Nu chapter (Purdue University) (2016).
- 4) Cleared GATE in Chemistry (2015).
- 5) Purdue University International Student Travel Award (2015).
- 6) Student Awards for discounted registration DMC (2019).
- 7) Rajya Puraskar award by The Bharat Scouts & Guides (2006)

**Academic Career Goal:** Study fundamental and applied areas of molecular sciences. Lead a state-of-the-art academic research lab in the field of experimental chemical physics and high-resolution molecular spectroscopy with basic theoretical support. Collaborate with researchers from diverse fields.

### List of Publications:

#### **Publications as corresponding author**

- 1) Chirped-Pulse Fourier-Transform Millimeter-wave Rotational Spectroscopy of Furan in its  $\nu_{10}$  and  $\nu_{13}$  Excited Vibrational States. Mishra, P.\*; Hull, A. W.; Barnum, T. J.; McGuire, B. A.; Field, R. W., *J. Mol. Spectrosc.* 2022, **388**, 111686. [10.1016/j.jms.2022.111686](https://doi.org/10.1016/j.jms.2022.111686)

#### **Publications as 1st author**

- 2) Signatures of Reaction Mechanism Encoded in the Vibrational Population Distribution of Small Molecular Products: Photodissociation of Symmetric-Triazine Using 266 nm. Mishra, P.; Hull, A. W.; Coy, S. L.; Field, R. W.\*, *J. Phys. Chem Lett.* 2023, **14**, 3706. [10.1021/acs.jpcllett.3c00597](https://doi.org/10.1021/acs.jpcllett.3c00597)

- 3) Gas-phase pyrolysis of *trans* 3-pentenitrile: Competition between direct and isomerization-mediated dissociation. Mishra, P.; Fritz, S. M.; Herbers, S.; Mebel, A. M.\*; Zwier, T. S.\*, *Phys. Chem. Chem. Phys.* 2021, **11**, 6462. [10.1039/D1CP00104C](https://doi.org/10.1039/D1CP00104C)
- 4) Broadband rotational spectroscopy of *trans* 3-pentenitrile and 4-pentenitrile. Mishra, P.; Fritz, S. M.; Hays, B. M.; Mehta-Hurt, D. N.; Jawad, K. M.; Zwier, T. S.\*, *Phys. Chem. Chem. Phys.* 2019, **21**, 23651. [10.1039/C9CP04328D](https://doi.org/10.1039/C9CP04328D)
- 5) Conformational explosion: Understanding the complexity of short chain *para*-dialkylbenzene potential energy surfaces. Mishra, P.; Hewett, D. M.; Zwier, T. S.\*, *J. Chem. Phys.* 2018, **148**, 184304. [10.1063/1.5029373](https://doi.org/10.1063/1.5029373)
- 6) Does borazine-water behave like benzene-water? A matrix isolation infrared and *ab initio* study. Mishra, P.; Verma, K.; Bawari, D.; Viswanathan, K. S.\*, *J. Chem. Phys.* 2016, **144**, 234307. [10.1063/1.4953793](https://doi.org/10.1063/1.4953793)

#### Other publications

- 7) Jet-cooled phosphorescence excitation spectrum of the  $T_1(n,\pi^*) \leftarrow S_0$  transition of 4*H*-Pyran-4-one. Parsons, S. W.; Hucek, D. G.; Mishra, P.; Zwier T. S.; Drucker S., *J. Phys. Chem. A* 2023, **127**, 3636. [10.1021/acs.jpca.3c01059](https://doi.org/10.1021/acs.jpca.3c01059)
- 8) Detecting combustion intermediates via broadband chirped-pulse microwave spectroscopy. Fritz, S. M.; Mishra, P.; Wullenkord, J.; Fugazzi, P. G.; Kohse-Hinghaus, K.; Zwier, T. S.\*; Hansen, N.\*, *P. Combust. Inst.* 2021, **38**, 1761. [10.1016/j.proci.2020.06.169](https://doi.org/10.1016/j.proci.2020.06.169)
- 9) Local and global approaches to treat the torsional barriers of 4-methylacetophenone using microwave spectroscopy. Herbers, S.; Fritz, S. M.; Mishra, P.; Nguyen, H. V. L.\*; Zwier, T. S.\*, *J. Chem. Phys.* 2020, **152**, 074301. [10.1063/1.5142401](https://doi.org/10.1063/1.5142401)
- 10) Insights into the photoprotection mechanism of the UV filter homosalate. Holt, E. L.; Krokidi, K. M.; Turner, M. A. P.; Mishra, P.; Zwier, T. S.; Rodrigues, N. d. N.\*; Stavros, V. G.\* *Phys. Chem. Chem. Phys.* 2020, **22**, 15509. [10.1039/D0CP02610G](https://doi.org/10.1039/D0CP02610G)
- 11) The unusual symmetry of hexafluoro-*o*-xylene-A microwave spectroscopy and computational study. Herbers, S.\*; Fritz, S. M.; Mishra, P.; Kim, Y.; Slipchenko, L.; Zwier, T. S.\*, *J. Chem. Phys.* 2020, **152**, 064302. [10.1063/1.5142169](https://doi.org/10.1063/1.5142169)
- 12) Strong Field Coherence Breaking as a tool for identifying methyl rotor states in microwave spectra: 2-hexanone. Fritz, S. M.; Mishra, P.; Zwier, T. S.\*, *J. Chem. Phys. Comm.* 2019, **151**, 041104. [10.1063/1.5109656](https://doi.org/10.1063/1.5109656)

#### Publications submitted as the corresponding author

- 13) Propylbenzene(Water)<sub>n</sub>, n=2-4 Clusters: What Happens When a Short Aliphatic Chain is Introduced to the Prototypical Benzene(Water)<sub>n</sub>, n=2-4 System? Mishra, P.\*; Fisher, J. L. (Submitted to *Spectrochim. Acta A*)

#### Manuscripts in preparation:

- 14) Collisional relaxation of low-frequency vibrational modes of small molecules in a pulsed seeded supersonic jet – Part 1: Qualitative lessons from a map of the parameter space for helium carrier gas. Mishra, P.; Hull, A. W.; Coy, S. L.; Muentner, J. S.; Field, R. W.
- 15) Collisional relaxation of low-frequency vibrational modes of small molecules in a pulsed seeded supersonic jet – Part 2: Qualitative lessons from the variation of the collision partner. Mishra, P.; Hull, A. W.; Coy, S. L.; Muentner, J. S.; Field, R. W.
- 16) Electronic spectroscopy of 2-ethylanthracene. Mishra, P.; Zwier, T.S.
- 17) Broadband rotational spectroscopy of pentanal and 2-pentenal. Fritz, S. M.; Mishra, P.; Zwier, T. S.
- 18) Broadband Rotational Spectroscopy of Nitrile Chain Conformations: 4-Pentynenitrile and Glutaronitrile. Mishra, P.; Fritz, S. M.; Hays, B. M.; Mehta-Hurt, D. N.; Jawad, K. M.; Zwier, T. S.\*

#### Ongoing Projects as Collaborator:

- 1) Modelling vibrational cooling in a seeded Helium supersonic jet.
- 2) Chirped-pulse millimeter wave spectroscopy of Dihydropyran series of molecules.
- 3) Chirped-pulse millimeter wave spectroscopy of Ethylvinylether.
- 4) Chirped-pulse millimeter wave spectroscopy of the bridged compound norbornene and its derivatives.
- 5) Studying the stacking tendency of Dianthrylethanes.

#### Scientific Contributions:

- 1) Involved in writing the US Department of Energy proposal titled “Signatures of Reaction Mechanisms in the Vibrational Population Distribution of Reaction Products” with Prof. Robert W. Field. Proposal was funded (Award number: SC0021580).
- 2) Designed and built Chirped-pulse rotational spectrometer at Massachusetts Institute of Technology, MA, USA.

- 3) Used effective measurement of vibrational population distribution of polar molecules to study collision kinetics and reaction dynamics using the multiplexed, high-resolution Chirped-pulse rotational spectroscopy.

#### **Other Scientific Experiences:**

- 1) Visited the Patterson Lab (Department of Physics) at the University of California, Santa Barbara, CA, USA to learn about cryogenic buffer gas spectroscopy and microwave 3-wave mixing for enantiomer detection. (2022)
- 2) Mentored a Graduate student and a postdoc in the McGuire group at MIT on Chirped-pulse rotational spectroscopy, which will result in at least 2 publications.
- 3) Involved in building molecular dynamics imaging instruments at the University of Ottawa, ON, Canada (2023).
- 4) Was a judge for 'Rao Prize' at the International Symposium on Molecular Spectroscopy (ISMS-2022).
- 5) Coordinated events of the 'CHEM-WEEK', organized by the Curie Club of IISER, Mohali. (2012).
- 6) Environment, Health, and Safety (EHS) representative of the Field group at MIT (2022).

#### **Laboratory Skills and Technical Expertise:**

- 1) Laser spectroscopy (vibrational and electronic) spanning infrared and ultraviolet regions.
- 2) Chirped-pulse spectroscopy (rotational) spanning microwave and millimeter wave regions.
- 3) Cooling techniques: supersonic jet expansion, cryogenic matrix isolation.
- 4) Multiple resonance spectroscopic techniques across rotational, vibrational and electronic regimes.
- 5) Mass spectrometry and charged particle optics coupled with spectroscopic techniques.
- 6) Vacuum systems.
- 7) Basic computational and simulation techniques: Gaussian, PGOPHER, MATLAB.

#### **Teaching Experience:**

- 1) Teaching assistant (TA)-Undergraduate chemistry lab (BS level, 1 semester) in IISER Mohali.
- 2) TA-Analytical chemistry lab (MS level, 1 semester) in IISER Mohali.
- 3) TA-Undergraduate General chemistry recitation and lab (3 semesters) at Purdue University.
- 4) TA-Undergraduate Physical chemistry lab (1 semester) at Purdue University.

#### **Conference and Workshop Participation:**

- 1) Talks delivered:  
International Symposium on Molecular Spectroscopy (ISMS) 2017, 2018, 2019, 2022  
Future of Chemistry (14<sup>th</sup> symposium) Invited talk 2023  
International Conference on Molecular Energy Transfer in Complex Systems (iComet) 2023
- 2) Presented poster:  
Dynamics of Molecular Collisions XXVII (DMC-2019),  
Gordon Research Seminar (GRS-2022) and Gordon Research Conference (GRC-2022)
- 3) Participated:  
Vigyan Jyoti Shibir (National Science Camp) (Vijyoshi-2009), ISMS-2016, ISMS-2021  
International Symposium on Molecular Spectroscopy (ISMS) 2016, 2021  
U.S. Department of Energy (DOE)- 41<sup>st</sup> Annual Principal Investigator's Meeting 2022,  
Schawlow-Townes Symposium on Photonics 2023

#### **Summer Internships:**

- 1) 2010: S. Ganesan group (Anna University, Chennai)
- 2) 2011: K. S. Viswanathan group and Summer Training in Physics and Chemistry (STIPAC) (IGCAR, Kalpakkam)
- 3) 2012: R. Adhikari group (Institute of Mathematical Science, Chennai)
- 4) 2013: A. Bhattacharya group (Indian Institute of Science, Bengaluru)
- 5) 2014: K. S. Viswanathan group (Indian Institute of Science Education and Research, Mohali)

#### **Presented research work at the following academic institutions:**

- 1) Spectroscopy division, Department of Chemistry, University of Southern California, Los Angeles, USA.
- 2) Department of Physics, Indian Institute of Technology (IIT) Madras, Chennai, India.
- 3) Chemical Dynamics meeting, Department of Chemistry, Indian Institute of Science, Bangalore, India.
- 4) Indian Institute of Science Education and Research, Tirupati, India.