Dr. Sabyashachi Mishra

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Education and Employments

Since 2020	Associate Head	Centre for Computational and Data Sciences, IIT Kharagpur, India.
Since 2018	Associate Professor	Department of Chemistry, IIT Kharagpur, India.
2012 - 2018	Assistant Professor	Department of Chemistry, IIT Kharagpur, India.
2009 - 2012	Postdoc	Department of Biochemistry, University of Zurich, Switzerland.
2007 - 2009	Postdoc	Department of Chemistry, University of Basel, Switzerland.
2003 - 2006	PhD (Chemistry)	Department of Chemistry, Technical University of Munich, Germany.
2001 - 2003	MSc (Chemistry)	School of Chemistry, University Hyderabad, India.
1998 - 2001	BSc (Chemistry Hons)	Ravenshaw College, Cuttack, India.

Teaching

Courses taught in IIT Kharagpur

- Preparatory Chemistry (CY00002)
- Chemistry (CY11001)
- Chemistry Lab (CY19001)
- Physical Chemistry Laboratory II (CY39001)
- Introduction to Computational Chemistry (CY40014)
- Introduction to Quantum Chemistry and Spectroscopy (CY40019)
- Biochemical Techniques Laboratory (CY49006)
- Advanced Quantum Chemistry (CY60105)
- Chemical Bonding and Reactivity (CY61010)
- Molecular Spectroscopy and Molecular Structure (CY61044)
- Quantum Methods in Molecular Simulations (TS62002)

Research Supervision

- PhD Thesis Supervision: 3 PhD Completed, 2 Senior Research Fellows, 5 Junior Research Fellows.
- Postdoctoral Fellow: 1
- MSc Thesis Supervision: 12 completed.

Awards

- Member of the National Academy of Sciences India (NASI), 2020.
- International Strategic Fund Award of University of Bristol, UK, 2019.
- Odisha Young Scientist Award, 2018 by the Government of Odisha.
- Faculty Excellence Award of IIT Kharagpur, 2017.
- Young Associate of the Indian Academy of Sciences, Bangalore, 2016.
- Amongst the teachers of IIT Kharagpur with best teaching feedback for the Academic Years 2018-2014.
- Ramanujan Fellowship of the Department of Science and Technology, India, 2012.
- DST INSPIRE Faculty Award from the Department of Science and Technology, India, 2012.

- *Forschungskredit* (Research Credit) Grant Award by University of Zurich, Switzerland, 2010
- Extra-mural research grant from the Holcim foundation (2010).
- Extra-mural research grant from the Novartis foundation (2009).
- Short-term research visit grant from the European Cooperation in Science and Technology, 2005.
- University Gold medals for securing top rank in M.Sc. Chemistry, 2003 (University of Hyderabad) and B.Sc. Chemistry Hons., 2001 (Ravenshaw College).

Sponsored Projects

- (2019–2022) Council of Scientific and Industrial Research, Govt. of India, "Nonadiabatic Dynamics of Spin Crossover in Transition Metal Complexes", as Principal Investigator.
- (2019–2021) SPARC, MHRD, Govt. of India, "Perylene-based Supramolecular Polymers: from Controlled Structure to Controlled Function", as Co-Principal Investigator.
- (2016–2019) Science and Engineering Research Board, Govt. of India, "Conformational Dynamics, Substrate Specificity and Catalytic Mechanism of Lipoxygenases", as Principal Investigator.
- (2014–2017) Sponsored Research and Industrial Consultancy, IIT Kharagour, "Chemical Dynamics and Relativistic Effects in the Excited States", as Principal Investigator.
- (2012–2017) Department of Science and Technology, Govt. of India, "Catalytic Hydrolysis by a Microbial Enzyme with Potential as an Antibiotic Target: A Computational Study", as Principal Investigator.
- (2012–2015) Sponsored Research and Industrial Consultancy, IIT Kharagour, "Cooperativity in Ligand Migration in a Dimeric Microbial Hemoglobin", as Principal Investigator.

Presentation at Conferences/Symposia

- Recent Trends in Molecular Magnetism, IISER Bhopal, 12/2019.
- Recent Advances in Molecular Magnetism, IIT Kharagpur, 11/2019.
- Application of Computational Methods in Modern Science, Bajkul Milani College, West Bengal, 09/2019.
- Guest Lecture on Multi-scale Simulation of Enzymatic Action, School of Chemistry, University of Bristol, UK, 07/2019.
- Symposium on Materials Simulation from Classical to Quantum, IIT Kharagpur, 05/2019.
- in National Symposium in Chemitry, Bhadrak College, Bhadrak, 03/2019.
- Guest Lecture at University of Hyderabad, Hyderabad, 07/2018.
- Conference on Electronic Spectroscopy, Structure and Dynamics, IACS Kolkata, 02/2018.
- National Symposium on Convergence of Chemistry and Materials, BITS Hyderabad, 12/2017.
- QM/MM Methods and Applications, Manchester, UK, 09/2017.
- Kaleidoscope, A Discussion Meeting in Chemistry, Goa, India, 07/2017.
- CRSI ACS Meeting, IICT Hyderabad, India, 07/2017.
- Modelling of Chemical and Biological Reactivity (MCBR-5), CLRI Chennai, India, 02/2017.
- Theoretical Chemistry Symposium, University of Hyderabad, India, 12/2016.
- Brainstorming meeting of the National Supercomputing Mission (NSM), Centre for Development of Advanced Computing, Pune, 04/2016.
- The World Academy of Science Young Scientists Conference, JNCASR Bangalore, 12/2015.
- Physical and Biophysical Chemistry: Theory and Experiment, IIT Mumbai, 12/2015.
- International Congress of Quantum Chemistry, Beijing, 06/2015.
- Workshop on Computational Modelling, IACS Kolkata, 10/2014.

- Symposium on Chemistry with Computers, IIIT Hyderabad, 01/2014.
- Theoretical Chemistry Symposium, IIT Guwahati, India, 12/2012.

Institute/Departmental Responsibilities

- Convener/Organizer: TEQIP Workshop on Applications of Computers in Chemistry (2020); Functional Smart and Supramolecular Materials Symposium (2020); Recent Advances in Molecular Magnetism Symposium (2019); Advances in Functional Materials Symposium (2019), Electronic Structure and Dynamics Symposium (2018); National Science Day Lecture (2017); Sir P. C. Ray Lecture (2016).
- Continuous Evaluation Committee Member of IIT Kharagpur (2020-).
- Planning and Coordination Committee Member of IIT Kharagpur (2020-).
- Core Committee Member of the Centre for Computational and Data Sciences, IIT Kharagpur (2017-2020).
- Member of Publication Sub Committee for Annual Convocation of IIT Kharagpur (2016-2019).
- Program Officer, NSO-H&F (2015-2018).
- Faculty Advisor for MSc Chemistry students (2015-2020).
- Faculty In-charge, Training and Placement, Department of Chemistry (2019-2020).
- Chemistry Department Research Scholar Coordinator (Since 2020).
- Chemistry Department HPC Instrument Co-Incharge (Since 2015).

List of Publications

1. Aging Dependent Morphological Crystallinity Determines Membrane Activity of L-Phenylalanine Self-Assembles
   P. Banerjee, K. Rajak, P. Nandi, S. Pal, M. Ghosh, **S. Mishra***, and N. Sarkar
   J. Phys. Chem. Lett. 11 (2020) 8585-8591.
2. Role of Substituents at 3-position of Thienylethynyl Spacer on Electronic Properties in Diruthenium(II) Organometallic Wirelike Complexes
   S. S. Roy S. Roy Chowdhury, **S. Mishra***, and S. K. Patra
   Chem. Asian J. (2020) In press.
3. Flipped Regiospecificity in L434F Mutant of 8-Lipoxygenase
   V. K. Mishra and **S. Mishra***. Phys. Chem. Chem. Phys. 22 (2020) 16013-16032.
4. Correlation Effects in the Photoelectron Spectrum and Photoionization Dynamics of OsO_4
   S. Manna and **S. Mishra***. Phys. Chem. Chem. Phys. 22 (2020) 628-641.
5. C3-Thioester/-Ester Substituted Linear Dienones: A Pluripotent Molecular Platform for Diversification via Cascade Pericyclic Reactions
   A. Bankura, S. Naskar, S. Roy Chowdhury, R. Maity, **S. Mishra***, and I. Das. Adv. Synth. Catal. 362 (2020) 3604-3612.
6. Through Bond Energy Transfer (TBET)-operated Fluoride Ion Sensing via Spirolactam Ring Opening of a Coumarin-Fluorescein Bichromophoric Dyad
   S. Pradhan, V. K. Mishra, N. Murmu, S. Mishra, and S. Sahu. RSC Adv. 10 (2020) 28422-28430.
7. On the Origin of Regio- and Stereospecific Catalysis by 8-Lipoxygenase
   V. K. Mishra and **S. Mishra***. J. Phys. Chem. B 123 (2019) 10605-10621.

8. Light-Induced Spin Crossover in an Intermediate-Spin Penta-Coordinated Iron(III) Complex
   S. Roy Chowdhury and **S. Mishra***. J. Phys. Chem. A 123 (2019) 9883-9892.
9. Spin-orbit vibronic coupling in $^4\Pi$ states of linear triatomic molecules.
   L. V. Poluyanov, W. Domcke, and **S. Mishra***. J. Chem. Phys. 151 (2019) 134103.
10. QM/MM-MD Simulation of the Catalytic Hydrolysis of L-Captopril by Microbial Enzyme DapE.
    D. Dutta, V. K. Mishra, and **S. Mishra***. J. Ind. Chem. Soc. 96 (2019) 767-774. Invited article for a special issue on "Theoretical Chemistry"
11. A Novel PEGylated Block Copolymer in New Age Therapeutics for Alzheimer's Disease.
    S. Som Chaudhury, A. Sannigrahi, M. Nandi, V. K. Mishra, P. De, K. Chattopadhyay, **S. Mishra**, J. Sil, and C. Das Mukhopadhyay. Molecular Neurobiology 56 (2019) 6551-6565.
12. Visible-Light-Activated Divergent Reactivity of Dienones: Dimerization in Neat Conditions and Regioselective E to Z Isomerization in the Solvent.
    S. Naskar, S. Roy Chowdhury, S. Mondal, D. K. Maiti, **S. Mishra***, and I. Das. Org. Lett. 21 (2019) 1578-1582.
13. Synthesis, Structure, Electrochemical and Spectroscopic Properties of Hetero-Bimetallic Ru(II)/Fe(II)-Alkynyl Organometallic Complexes.
    A. Sil, U. Ghosh, V. K. Mishra, **S. Mishra***, and S. K. Patra. Inorg. Chem. 58 (2019) 1155-1166.
14. Ab Initio Investigation of Magnetic Anisotropy in Intermediate Spin Iron(III) Complexes.
    S. Roy Chowdhury and **S. Mishra***. J. Chem. Phys. 149 (2018) 234302.
15. Vibronic Structures and Photoelectron Angular Distribution in the Photoelectron Spectrum of ICN.
    S. Manna and **S. Mishra***. J. Chem. Phys. 149 (2018) 204308.
16. Electronic Structure and Photoelectron Spectroscopy of Manganese Dihalides from Quantum Chemical Methods and Dyson Orbitals.
    S. Roy Chowdhury, S. Manna, and **S. Mishra***. Chem. Phys. 515 (2018) 513-520.
17. L-Captopril and its Derivatives as Potential Inhibitors of Microbial Enzyme DapE: A Combined Approach of Drug Repurposing and Similarity Screening.
    D. Dutta and **S. Mishra***. J. Mol. Graphics Modell. 84 (2018) 82-89.
18. Diruthenium(II)-capped Oligothienylethynyl Bridged Highly Soluble Organometallic Wires Exhibiting Long-range Electronic Coupling.
    S. Roy, A. Sil, D. Giri, S. Roy Chowdhury, **S. Mishra***, and S. K. Patra. Dalton Trans. 47 (2018) 14293-14303.
19. Synthesis, Structure, and Photophysical and Electrochemical Properties of Ru(II) Complexes of Arylene-vinylene Terpyridyl Conjugates.
    A. Sil, S. Roy Chowdhury, **S. Mishra***, and S. K. Patra. Dalton Trans. 47 (2018) 9877-9888.
20. Active Site Dynamics in the Substrate Hydrolysis Catalyzed by DapE Enzyme and Its Mutants from Hybrid QM/MM Molecular Dynamics Simulations.
    D. Dutta and **S. Mishra***. J. Phys. Chem. B 121 (2017) 7075-7085.
21. Heavy Ligand Atom Induced Large Magnetic Anisotropy in Mn(II) Complexes.
    S. Roy Chowdhury and **S. Mishra***. Phys. Chem. Chem. Phys. 19 (2017) 16914-16922.
22. Role of Ligand Field, Structural Distortion, and Conformational Dynamics in the Magnetic Anisotropy of Linear Co(II) Complexes.
    S. Roy Chowdhury and **S. Mishra***. Eur. J. Inorg. Chem. (2017) 659-668.
23. Synthesis and Studies on Gelation Ability of Phenol Based Maleate Amphiphile and its Application in

Nutraceutical Release.
B. A. Kumar, S. Roy Chowdhury, **S. Mishra** and R. R. Nayak. Colloids Surf. A 537 (2017) 310-317.

24. Loss of Catalytic Activity in the E134D, H67A, and H349A Mutants of DapE: Mechanistic Analysis with QM/MM Investigation.
D. Dutta and **S. Mishra***. J. Phys. Chem. B 120 (2016) 11654-11664.
25. Structural and Mechanistic Insight into the Substrate Binding from the Conformational Dynamics in Apo and Substrate-Bound DapE Enzyme.
D. Dutta and **S. Mishra***. Phys. Chem. Chem. Phys. 18 (2016) 1671-1680.
26. The Role of Spin-Orbit Coupling in the Double-Ionization Photoelectron Spectra of XCN2+ (X = Cl, Br, and I).
S. Manna and **S. Mishra***. J. Phys. Chem. A 120 (2016) 1554-1561.
27. QM/MM Simulation of the Amide-I Band in the Raman Spectrum of Insulin.
B. Tah, D. Dutta, P. Pal, G. B. Talapatra, and **S. Mishra***. Mol. Phys. 114 (2016) 1939-1951.
28. Specific Inhibition of beta-Secretase Processing of the Alzheimer Disease Amyloid Precursor Protein.
S. B. Halima, **S. Mishra**, K. M. Raja, M. Willem, A. Baici, K. Simons, O. Brustle, P. Koch, C. Haass, A. Caflisch, L. Rajendran. Cell Reports, 14 (2016) 1-15.
29. Carboxylate Coordination Assisted Aggregation for Quasi-Tetrahedral and Partial-Dicubane [Cu4] Coordination Clusters.
T. S. Mahapatra, A. Bauza, D. Dutta, **S. Mishra**, A. Frontera, and D. Ray. ChemistrySelect 1 (2016) 64-74.
30. The Structural and Energetic Aspects of Substrate Binding and the Mechanism of Action of the DapE-Encoded N-Succinyl-L,L-Diaminopimelic Acid Desuccinylase (DapE) Investigated Using A Hybrid QM/MM Method.
D. Dutta and **S. Mishra***. Phys. Chem. Chem. Phys. 16 (2014) 26348.
31. Interaction of Insulin with Anionic Phospholipid (DPPG) Vesicles.
B. Tah, P. Pal, **S. Mishra**, and G. B. Talapatra. Phys. Chem. Chem. Phys. 16 (2014) 3987.
32. Quantum-Mechanical DFT Calculation Supported Raman Spectroscopic Study of Some Amino Acids in Bovine Insulin.
B. Tah, P. Pal, S. Roy, D. Dutta, **S. Mishra**, M. Ghosh, and G. B. Talapatra. Spectrochim. Acta A 129 (2014) 345.
33. Structural Diversity of Copper(I) Complexes Formed by Pyrrole- and Dipyrrolylmethane-based Diphosphine Ligands with Cu-X $\cdots$ HN Hydrogen Bonds.
S. Kumar, G. Mani, D. Dutta, and **S. Mishra**. Inorg. Chem. 53 (2014) 700.
34. Dynamics in the active site of β-secretase: A network analysis of atomistic simulations.
S. Mishra* and A. Caflisch. Biochemistry 50 (2011) 9328.
35. Quantitative analysis of ligand migration from transition networks.
S. Mishra and M. Meuwly. Biophys. J. 99 (2010) 3969.
36. Atomistic simulation of NO dioxygenation in group I truncated hemoglobin.
S. Mishra and M. Meuwly. J. Am. Chem. Soc. 132 (2010) 2968.
37. Reactive Processes with Molecular Dynamics Simulations.
S. Mishra and M. Meuwly. In Kinetics and Dynamics From Nano to Bio Scale. Springer series on: Challenges and Advances in Computational Chemistry and Physics, Volume 12 (2010) Chapter 5. ISBN 978-90-481-3033-7.

38. Nitric oxide dynamics in truncated hemoglobin: Docking sites, migration pathways, and vibrational spectroscopy from molecular dynamics simulations.
    S. Mishra and M. Meuwly. Biophys. J. 96 (2009) 2105.
39. Structural and spectroscopic study of the excited electronic states of silver dihalides by quantum chemical methods.
    S. Mishra*. Phys. Chem. Chem. Phys. 10 (2008) 3987.
40. Renner-Teller and spin-orbit vibronic coupling effects in linear triatomic molecules with a half-filled π shell.
    I. Sioutis, **S. Mishra**, L. V. Poluyanov, and W. Domcke. J. Chem. Phys. 128 (2008) 124318.
41. A study of spin-orbit vibronic coupling effects in the $\tilde{A}^3\Pi$ state of CCX (X= O, S, Se) and CNY (Y= N, P, As).
    S. Mishra*, W. Domcke, and L. V. Poluyanov. Chem. Phys. Lett. 446 (2007) 256.
42. Theoretical calculation of photodetachment spectra of $XAuY^-$, (X, Y= Cl, Br, and I).
    S. Mishra*. J. Phys. Chem. A 111 (2007) 9164.
43. Spin-orbit vibronic coupling in $^3\Pi$ states of linear triatomic molecules.
    S. Mishra*, L. V. Poluyanov, and W. Domcke. J. Chem. Phys. 126 (2007) 134312.
44. Quasistationary upper-well states of E$\times$E Jahn-Teller systems with spin-orbit coupling.
    L. V. Poluyanov, **S. Mishra***, and W. Domcke. Chem. Phys. 332 (2007) 243.
45. Quasiclassical calculation of the vibronic energy levels of the E$\times$E Jahn-Teller effect including spin-orbit coupling.
    L. V. Poluyanov, **S. Mishra**, and W. Domcke. Mol. Phys. 105 (2007) 1471.
46. Calculation of vibronic structure of the $\tilde{X}\ ^2\Sigma^+ - \tilde{A}\ ^2\Pi$ photodetachment spectra of $CCCl^-$ and $CCBr^-$.
    S. Mishra*, V. Vallet, L. V. Poluyanov, and W. Domcke. J. Chem. Phys. 125 (2006) 164327.
47. Study of strong $\Sigma - \Pi$ and spin-orbit vibronic coupling effects in linear triatomic molecules.
    S. Mishra*, L. V. Poluyanov, and W. Domcke. Chem. Phys. 327 (2006) 457.
48. Calculation of the vibronic structure of the $\tilde{X}\ ^2\Pi$ photoelectron spectra of XCN, X= F, Cl, and Br.
    S. Mishra*, V. Vallet, L. V. Poluyanov, and W. Domcke. J. Chem. Phys. 124 (2006) 044317.
49. Importance of spin-orbit coupling for the assignment of the photodetachment spectra of AuX_2^-, X= Cl, Br, and I.
    S. Mishra, V. Vallet, and W. Domcke. ChemPhysChem 7 (2006) 723.
50. The relativistic E$\times$E Jahn-Teller effect revisited.
    W. Domcke, **S. Mishra**, and L. V. Poluyanov. Chem. Phys. 322 (2006) 405.
51. Spectroscopic effects of first-order relativistic vibronic coupling in linear triatomic molecules.
    S. Mishra, V. Vallet, L. V. Poluyanov, and W. Domcke. J. Chem. Phys. 123 (2005) 124104.