Dr. Sabyashachi Mishra

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Education and Employments

Since 2018	Associate Professor	Department of Chemistry, IIT Kharagpur, India.
2020 - 2021	Associate Head	Centre for Computational and Data Sciences, 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.

Research Interest

Broad Research Interest: Computational Chemistry in Molecular Biology and Molecular Physics, with particular attention to,

- Bio-molecular Simulations and QM/MM Modelling of Enzyme Catalysis
- Electronic Structure, Spectroscopy, and Magnetism with Multi-Reference Methods
- Electronic Structure Calculations in Complex Systems
- Quantum Computing in Chemistry

Research Supervision

- PhD Thesis Supervision: 5 awarded, 5 SRF, 2 PMRF, 2 JRF.
- MSc Thesis Supervision: 20 completed; 3 in progress.

PhD Theses Supervised

- Dr. Atanuka Paul: Hybrid QM/MM Investigation of the Role of Metal Ions in the Substrate Binding and Catalysis of the Microbial Enzyme DapE (2023).
- Dr. Vipin Kumar Mishra: Computational Study of Regio– and Stereo–Selective Catalysis by 8–Lipoxygenase (2021).
- Dr. Soumitra Manna: Photoelectron Spectra and Photoionization Dynamics of Small Molecules with Heavy Atoms (2020).
- Dr. Sabyasachi Roy Chowdhury: Magnetic Anisotropy and Light–Induced Spin Crossover in Transition Metal Complexes (2019).
- Dr. Debodyuti Dutta: Catalytic Action of Microbial Enzyme DapE and Rational Design of its Potential Inhibitors (2017).

Sponsored Projects

- (2022–2025) Science and Engineering Research Board, Govt. of India, "Coordination Induced Spin Crossover in Transition Metal Complexes", as Principal Investigator (INR 52.5 Lakhs).
- (2019–2022) Council of Scientific and Industrial Research, Govt. of India, "Nonadiabatic Dynamics of Spin Crossover in Transition Metal Complexes", as Principal Investigator (INR 6.3 Lakhs).
- (2019–2021) SPARC, MHRD, Govt. of India, "Perylene-based Supramolecular Polymers: from Controlled

Structure to Controlled Function", as Co-Principal Investigator (INR 65.4 Lakhs).
- (2016–2019) Science and Engineering Research Board, Govt. of India, "Conformational Dynamics, Substrate Specificity and Catalytic Mechanism of Lipoxygenases", as Principal Investigator (INR 55 Lakhs).
- (2014–2017) Sponsored Research and Industrial Consultancy, IIT Kharagpur, "Chemical Dynamics and Relativistic Effects in the Excited States", as Principal Investigator (INR 21 Lakhs).
- (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 (INR 73 Lakhs).
- (2012–2015) Sponsored Research and Industrial Consultancy, IIT Kharagpur, "Cooperativity in Ligand Migration in a Dimeric Microbial Hemoglobin", as Principal Investigator (INR 5 Lakhs).

Teaching

Courses taught at IIT Kharagpur

- Preparatory Chemistry (CY00002)
- Chemistry (CY11001)[1]
- Chemistry Laboratory (CY19001)
- Physical Chemistry Laboratory II (CY39001)
- Introduction to Computational Chemistry (CY40014)
- Introduction to Quantum Chemistry and Spectroscopy (CY40019)
- Molecular Thermodynamics and Kinetics (CY41012)
- 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/CD61006)
- Essential Tools for Scientific Computing (CD61203)

Online Courses

- IIT PAL Chemistry (8 hours), Swayam Prabha, DTH.
- Quantum Chemistry and Spectroscopy (30 hours), Swayam Prabha, DTH.
- Approximate Methods in Quantum Chemistry (20 hours), NPTEL.

Recognitions

- Review Editor for Theoretical and Computational Chemistry Section of Frontiers in Chemistry, 2021.
- 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 2014-2018.
- 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).

Recognitions for Group Members

- Harshdeep Singh: Best Poster Prize at the Theoretical Chemistry Symposium (TCS), IIT Madras (Dec 2023).
- Sunita Muduli: Best Poster Prize at the National Conference on "Recent Advances in Chemistry: Theoretical and Computational Aspects, NIT Meghalaya (Nov 2022).
- Kishan Kumar Dakua: Best Poster Prize at the Current Trends in Theoretical Chemistry, BARC Mumbai (Sep 2022).
- Soumyajit Karmakar: Prime Minister's Research Fellowship (Oct 2022).
- Harshdeep Singh: Prime Minister's Research Fellowship (May 2022).
- Sunita Muduli: Best Poster Prize at the National Conference on Molecular Modelling and Simulations, Vellore Institute of Technology Bhopal (Feb 2022).
- Soumyajit Karmakar: Best Mini Oral Presentation Prize in the MedChem, IIT Madras (Dec 2021).
- Harshdeep Singh: First Prize in the Qiskit Fall Fest, Ahmedabad University (Oct 2021).
- Vipin Kumar Mishra: Professor Santi Ranjan Palit Memorial Prize, Indian Chemical Society, Kolkata (Dec 2020).
- Vipin Kumar Mishra: Young Scientist Prize in the International Conference on Sustainable Energy and Environmental Challenges, G. H. Raisoni University, Madhya Pradesh (Jul 2020).
- Sabyasachi Roy Chowdhury: Best Poster Prize in the Recent Advances in Molecular Magnetism, IIT Kharagpur (Nov 2019).
- Soumitra Manna: Best Poster Prize in the 9th Conference of the Asia-Pacific Association of Theoretical and Computational Chemistry, Sydney, Australia (Oct 2019).
- Sabyasachi Roy Chowdhury: Best Poster Prize in the Modern Trends in Molecular Magnets, IIT Bombay (May 2016).

Presentation at Conferences/Symposia

- Spectroscopy and Dynamics of Molecules and Clusters (SDMC 2024), IIT Guwahati, 02/2024.
- Workshop on High-Performance Computing in Bioinformatics, CCDS IIT Kharagpur, 02/2024.
- Theoretical Chemistry Symposium, IIT Madras, 12/2023.
- Structure and Dynamics: Spectroscopy and Scattering (SDSS-2023), IACS Kolkata, 10/2023.
- From Proteins to Networks, University of Zurich, 03/2023.
- UGC-HRDC Refresher Course in Chemistry, Pt Ravishankar Shukla University, Chhatisgarh, 07/2022.
- Theoretical Chemistry Symposium, IISER Kolkata, 12/2021.
- NSM-IIT KGP Workshop on Simulation Methods in Scientific Computing, IIT Khragpur, 06/2021.
- 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.
- National Symposium in Chemistry, 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

- Outreach: Disaster Management Workshop (2023) as NSO Coordinator, Mental Health Awareness Workshop (2023) as NSO Coordinator, International Conference on Modern Trends in Molecular Magnetism (2022, with Prof. P. K. Chakraborty), TEQIP Workshop on Applications of Computers in Chemistry (2020, with Prof. A. Ayyappan); Functional Smart and Supramolecular Materials Symposium (2020, with Prof. S. K. Patra); Recent Advances in Molecular Magnetism Symposium (2019, with Prof. P. K. Chakraborty); Advances in Functional Materials Symposium (2019, with Prof. A. Pathak-Mohanty, Prof. D. Dhara), Electronic Structure and Dynamics Symposium (2018, with Prof. A. Ayyappan); National Science Day Lecture (2017, with Prof. S. Taraphder); Sir P. C. Ray Lecture (2016, with Prof. R. Samanta).
- Institute Level Responsibility: Program Coordinator (Since 2022); Associate Head, CCDS (2020-2021); Program Officer, NSO-H&F (2015-2018); Member of Publication Sub Committee for Annual Convocation of IIT Kharagpur (2016-2022); Instructor for the Training Program on Moodle Software for IIT Kharagpur Faculty (2020); Continuous Evaluation Committee Member of IIT Kharagpur (2020); Planning and Coordination Committee Member of IIT Kharagpur (2020).
- Department of Chemistry Faculty Advisor for MSc Chemistry students (2015-2020); Website in-charge (Since 2015); Dept Examination In-Charge (Since 2022); Faculty in-charge, Training and Placement (2019-2020); Faculty in-charge, Departmental UG Representative Election 2019; Member, Department Administrative Committee (2017-2019); Re- search Scholar Coordinator (2020-2022); HPC Instrument Co-in-charge (Since 2015); Seminar in-charge (2016-2018); PhD Student Recruitment in-charge (2016-2018); Timetable in-charge (2014-2016); 1st Year Chemistry Subject coordinator (2017-2018,2022-2023).
- Centre for Theoretical Studies: Research Scholar Coordinator (PDF in-charge, 2016-2019); Member, Purchase Committee (2019-2020).
- Centre for Computational and Data Sciences: Member, Core Committee (2017-2020); Member, HPC Advisory Committee (2019-2022); Associate Head (2020-2021).

Personal

Born	1982 in Cuttack, India.
Citizenship	Indian
Civil Status	Married with one son.

List of Publications

1. Design, Synthesis, and Characterization of Organometallic BODIPY-Ru(II) Dyads: Redox and Photophysical Properties with Singlet Oxygen Generation Capability
   A. Maity, V. K. Mishra, S. Dolai, **S. Mishra***, and S. K. Patra
   Inorg. Chem. (2024) In Press.
2. 2-Anilidomethylpyridine Derived Three-Coordinate Zinc Hydride: The Journey Unveils the Anilide Backbone's Reactive Nature
   C. Mandal, S. Joshi, S. Das, **S. Mishra***, and D. Mukherjee
   Inorg. Chem. 63 (2024) 739.
3. Highly Planar Pseudocapacitive Semiconducting Polymer Electrodes Toward Symmetric Supercapacitors with a Wide Range of Operating Potentials
   D. Patra, S.K. Pati, S. Muduli, **S. Mishra**, and S. Park
   Chem. Engg. J. 482 (2024) 149162.
4. Functionalized Carbon Nano-Onions as a Smart Drug Delivery System for the Poorly Soluble Drug Carmustine for the Management of Glioblastoma
   R. Majumder, S. Karmakar, **S. Mishra**, A. Mallick, C. Das Mukhopadhyay
   ACS Applied Bio Materials 7 (2024) 154-167.
5. The Interplay of Vibronic and Spin-Orbit Coupling in the Fluorescence Quenching in trans-dithionated PDI
   K. Dakua, K. Rajak, and **S. Mishra***
   J. Chem. Phys. 159 (2023) 114303.
6. Benchmarking of Different Optimizers in the Variational Quantum Algorithms for Applications in Quantum Chemistry
   H. Singh, S. Majumder, and **S. Mishra***
   J. Chem. Phys. 159 (2023) 044117.
7. Spin-State Energetics and Magnetic Anisotropy in Penta-coordinated Fe(III) Complexes with Different Axial and Equatorial Ligand Environments
   S. Joshi, S. Roy Chowdhury, and **S. Mishra***
   Phys. Chem. Chem. Phys. 25 (2023) 17680-17691.
8. Deciphering the Role of the Two Metal–Binding Sites of DapE Enzyme via Metal Substitution
   A. Paul and **S. Mishra***
   Comput. Biol. Chem. 103 (2023) 107832.
9. Ligands-Induced Open-Close Conformational Change during DapE Catalysis: Insights from Molecular Dynamics Simulations
   S. Muduli and **S. Mishra***
   Proteins: Struct. Funct. Bioinform. 91 (2023) 781-797.
10. The Coordinated Action of the Enzymes in the L-Lysine Biosynthetic Pathway and How to Inhibit it for Antibiotic Targets
    S. Muduli, S. Karmakar, and **S. Mishra***
    Biochim. Biophys. Acta 1867 (2023) 130320.
11. Excited-State Photophysics of Curcumin and its Modulation in Alkaline Non-Aqueous Medium
    M. Ghosh, S. Parida, H. Khatoon, N. Bera, **S. Mishra***, and N. Sarkar
    ChemPhysChem (2023) e202300174.
12. A coumarin-salicylidene based fluorescent chemodosimeter for sub-ppb level detection of aluminium ion

via metal ion induced hydrolytic cleavage of aldimine bond
S. K. Padhan, S. Muduli, N. Murmu, G. Sahoo, **S. Mishra***, and S. N. Sahu
J. Mol. Liq. 384 (2023) 122292.

13. Energy Storage Application of Conducting Polymers Featuring Dual Acceptors: Exploring Conjugation and Flexible Chain Length Effects
S. K. Pati, D. Patra, S. Muduli, **S. Mishra**, and S. Park
Small (2023) 2300689
14. Spirocyclic rhodamine B benzoisothiazole derivative: A multi-stimuli fluorescent switch manifesting ethanol-responsiveness, photo responsiveness, and acidochromism
B. Himabindu, M. Nath, **S. Mishra**, S. Jayanty
RSC Adv. 13 (2023) 5134-5148.
15. Synthesis and Application of Dual Electron-Deficient Featured Copolymers and their Sequential Fluorination for Ambipolar Organic Thin Film Transistors
D. Patra, X. Zhan, R. Linthoinganbi, S. Muduli, **S. Mishra**, Y. Liu, and S. Park
J. Mat. Chem. C 11 (2023) 1457-1463.
16. *(Book Chapter)* Electron Density in the Multiscale Treatment of Biomolecules,
S. Karmakar, S. Muduli, A. Paul, and **S. Mishra***
In Fundamentals of Electron Density. Wiley, (2023) In press.
17. *(Conference Paper)* On the Study of Partial Qubit Hamiltonian for Efficient Molecular Simulation Using Variational Quantum Eigensolvers
H. Singh, S. Mishra and S. Majumder
IEEE Xplore, 2023 International Conference on Quantum Technologies, Communications, Computing, Hardware and Embedded Systems Security (iQ-CCHESS), Kottayam, India, 2023, pp. 1-6.
18. Self-Assembling Behaviour of Perylene, Perylene Diimide, and Thionated Perylene Diimide Deciphered through Non-Covalent Interactions
S. Parida, S. K. Patra, and **S. Mishra***
ChemPhysChem 23, 23 (2022) 202200361.
19. Transition Metal Phthalocyanines as Redox Mediators in Li-O2 batteries: A Combined Experimental and Theoretical Study of the Influence of 3d Electrons in Redox Mediation
S. Mandal, R. Samajdar, S. Parida, **S. Mishra**, A. Bhattacharyya
ACS Appl. Mater. Interfaces 14 (2022) 26714-26723.
20. Identification of Potential Inhibitors Against FemX of Staphylococcus Aureus: A Hierarchial in-silico Drug Repurposing Approach
S. Rahman, K. Rajak, **S. Mishra***, and A. K. Das
J. Mol. Graph. Model. 115 (2022) 108215.
21. Spin-Vibronic Coupling in the Quantum Dynamics of a Fe(III) Trigonal Bipyramidal Complex
K. Dakua, K. Rajak, and **S. Mishra***.
J. Chem. Phys. 156 (2022) 134102.
22. Modulation of Electrochemical and Spectroscopic Properties in Ru(II)-Terpyridyl End-capped Homobimetallic Organometallic Complexes by Varying pi-Conjugated Organic Spacers
A. Sil, S. S. Roy, V. K. Mishra, S. N. Islam, **S. Mishra***, and S. K. Patra
Chemistry Select 7 (2022) e202200152.
23. Pomegranate Peel Polyphenols Prophylaxis against SARS-CoV-2 Main Protease by In-Silico Docking and Molecular Dynamics Study

M. Rakshit, S. Muduli, P. P. Srivastav, and **S. Mishra***
J. Biomol. Struct. Dynamics 40 (2022) 12917-12931.

24. Selective and Swift-responsive off-on Rhodamine B Based Chemosensors: Recognition of Multi-Metal Ions, On-site Sensing of Fe(III) in Water Samples and Bioimaging in Aqueous Media
H. Battula, S. Muduli, S. P. Bandi, S. Kapoor, **S. Mishra**, H. Aggarwal, V. Venuganti, S. Jayanty
J. Photochem. Photobiol. A 426 (2022) 113748.
25. 7,7-bis(N, N-diethylethylenediamino)-8,8-dicyanoquinodimethane: Effect of Ethyl Moiety on the Photophysical Property besides Thermal stability
A. Syed, **S. Mishra**, and S. Jayanty
J. Fluoresc. 32 (2022) 115-124.
26. Metal–Ion Promiscuity of Microbial Enzyme DapE at its Second Metal Binding Site
A. Paul and **S. Mishra***
J. Biol. Inorg. Chem. 26 (2021) 569-582.
27. Synthesis, structural characterization, and bonding analysis of two-coordinate copper(I) and silver(I) complexes of the pyrrole-based bis(phosphinimine): new metal-pyrrole ring $\pi-$interactions
V. K. Jha, S. Das, V. Subramaniyan, T. Guchhait, K. K. Dakua, **S. Mishra***, and G. Mani
Dalton Trans. 50 (2021) 8036-8044.
28. Distinct Tetracyanoquinodimethane Derivatives: Enhanced Fluorescence in Solutions and Unprecedented Cation Recognition in the Solid State
A. Syed, H. Battula, **S. Mishra*** and S. Jayanty
ACS Omega 4 (2021) 3090-3105.
29. Flipped Regiospecificity in L434F Mutant of 8-Lipoxygenase
V. K. Mishra and **S. Mishra***.
Phys. Chem. Chem. Phys. 22 (2020) 16013-16032.
30. 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.
31. 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.
32. Role of Substituents at 3-position of Thienylethynyl Spacer on Electronic Properties in Diruthenium(II) Organometallic Wire-like Complexes
S. S. Roy S. Roy Chowdhury, **S. Mishra***, and S. K. Patra
Chem. Asian J. 15 (2020) 3304-3313.
33. 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.
34. 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.
35. 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.

36. 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.
37. 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.
38. 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"
39. 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.
40. 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.
41. 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.
42. Ab Initio Investigation of Magnetic Anisotropy in Intermediate Spin Iron(III) Complexes.
S. Roy Chowdhury and **S. Mishra***.
J. Chem. Phys. 149 (2018) 234302.
43. Vibronic Structures and Photoelectron Angular Distribution in the Photoelectron Spectrum of ICN.
S. Manna and **S. Mishra***.
J. Chem. Phys. 149 (2018) 204308.
44. 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.
45. 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.
46. 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.
47. 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.

48. 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.
49. 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.
50. 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.
51. 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.
52. 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.
53. 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.
54. 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.
55. 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.
56. 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.
57. 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.
58. 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.

59. 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.
60. 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.
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