

Dr. Sabyashachi Mishra

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<http://www.chemistry.iitkgp.ac.in/fac/SM>

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 of 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: 10 (completed), 1 PMRF, 2 SRF, and 3 JRF.
- MS/BS Thesis Supervision: 25 completed; 4 in progress.

PhD Theses Supervised

10. Sanjukta Parida: Electronic Structure, Spectroscopy, and Charge Transport in Perylene-based Molecular Aggregates (2025).
9. Kishan Kumar Dakua: Excited-State Quantum Dynamics of Photophysical Processes in Organic Chromophores and Transition-Metal Complexes (2025).
8. Harshdeep Singh: Hybrid Quantum-Classical Algorithms for Quantum Chemistry (2025).
7. Dr. Shalini Joshi: Magnetic Anisotropy and Spin Crossover in Transition Metal Complexes with Multi-reference Electronic Structure Calculations (2025)
6. Dr. Sunita Muduli: Significance of Protein Dynamics in the Catalytic Activity of DapE and DapF Enzymes of the Lysine Biosynthetic Pathway (2024).
5. 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).
4. Dr. Vipin Kumar Mishra: Computational Study of Regio- and Stereo-Selective Catalysis by 8-Lipoxygenase (2021).
3. Dr. Soumitra Manna: Photoelectron Spectra and Photoionization Dynamics of Small Molecules with Heavy Atoms (2020).
2. Dr. Sabyasachi Roy Chowdhury: Magnetic Anisotropy and Light-Induced Spin Crossover in Transition Metal Complexes (2019).
1. Dr. Debodutti 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 Lipoygenases”, 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)
- 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)
- Modelling of Quantum Systems and Processes (CY62206)
- Quantum Methods in Molecular Simulations (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 the 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

- Soumyajit Karmakar: Poster Prize at Spins in Molecular Systems (SiMS), Kolkata (Dec 2025).
- Soumyajit Karmakar: Best Oral Presentation Prize at the Statistical Mechanics in Chemistry and Biology (SMCB), IIT Tirupati (Dec 2024).
- Moromi Nath: Best Flash Presentation Prize at the Advanced Functional Solids (AFS), IIT Kharagpur (Nov 2024).
- 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. Rasoni 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).

Hands-on Sessions/Workshops/Popular Science Lectures

- NSM Workshop on Quantum Computing, CCDS, IIT Kharagpur, 03/2025.
- SERB Workshop, IIT Kharagpur, 06/2024.
- Workshop on High-Performance Computing in Bioinformatics, CCDS IIT Kharagpur, 02/2024.
- Nurturance Program for NTS awardees, IIT Kharagpur, 12/2022
- UGC-HRDC Refresher Course in Chemistry, Pt Ravishankar Shukla University, Chhattisgarh, 07/2022.
- NSM-IIT KGP Workshop on Simulation Methods in Scientific Computing, IIT Kharagpur, 06/2021.
- TEQIP Workshop on "Applications of Computers in Chemistry", IIT Kharagpur, 02/2020
- Application of Computational Methods in Modern Science, Bajkul Milani College, West Bengal, 09/2019.
- National Symposium in Chemistry, Bhadrak College, Bhadrak, 03/2019.

Presentation at Conferences/Symposia

- Society for Physical Chemistry Meeting (SoPhyC-2025), IIT Patna, 10/2025.
- Asian and Oceanian Spectroscopy Conference (AOSC-2025), Goa, 09/2025.
- International Conference on Molecular Spin Qubits toward Quantum Computer and Sensor (ICMSQ2025), Sendai, Japan, 06/2025.
- Recent Advances in Modeling Rare Events (RARE), Khajuraho, 03/2025.
- Advances in Functional Solids, IIT Kharagpur, 11/2024.
- Modern Trends in Molecular Magnetism, IISc Bangalore, 11/2024.
- Society for Physical Chemistry Meeting, IIT Bombay, 10/2024.
- Kaleidoscope, A Discussion Meeting in Chemistry, Udaipur, 07/2024.
- Spectroscopy and Dynamics of Molecules and Clusters (SDMC 2024), IIT Guwahati, 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.
- Theoretical Chemistry Symposium, IISER Kolkata, 12/2021.
- Recent Trends in Molecular Magnetism, IISER Bhopal, 12/2019.
- Recent Advances in Molecular Magnetism, IIT Kharagpur, 11/2019.
- 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.
- 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

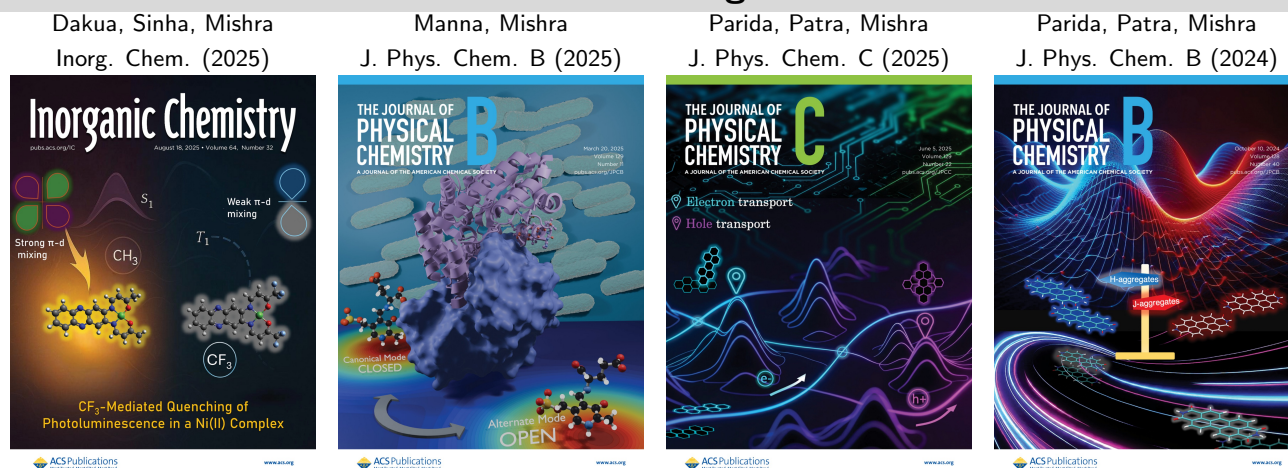
Institute/Departmental Responsibilities

- **Conferences and Symposia (Organized/Co-organized)**
 - Organizing Secretary for Modern Trends in Inorganic Chemistry (2024, with Prof. M. Bhattacharjee, C. R. Raj, and S. K. Patra).
 - Disaster Management Workshop (2023, 2024 as NSO H&F Coordinator)
 - Mental Health Awareness Workshop (2023 as NSO H&F 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 and 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 Responsibilities**
 - NSO Health & Fitness Program Coordinator (Since 2022)
 - Associate Head, Centre for Computational and Data Sciences (CCDS) (2020–2021)
 - Program Officer, NSO Health & Fitness (2015–2018)
 - Member, Publication Sub-Committee for Annual Convocation, IIT Kharagpur (2016–2025)
 - Instructor, Training Program on Moodle Software for IIT Kharagpur Faculty (2020)
 - Member, Continuous Evaluation Committee, IIT Kharagpur (2020)
 - Member, Planning and Coordination Committee, IIT Kharagpur (2020)
- **Department of Chemistry:** Faculty Advisor for MSc Chemistry students (2015-2020); Website in-charge (2015-2023); Dept Examination In-Charge (2022-2024); Faculty in-charge, Training and Placement (2019-2020); Faculty in-charge, Departmental UG Representative Election 2019; Member, Department Administrative Committee (2017-

2019); Research Scholar Coordinator (2020-2022); HPC Instrument Co-in-charge (2015-2023); 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).

Publications Featured as Journal Cover Page



List of Publications (Peer Reviewed Journal)

97. Quantum Computing for Molecular Systems:
Part I: Quantum Circuit and Measurement; Part II: Quantum Encoding; and Part III: Quantum Algorithms.
H. Singh, S. Majumder, and **S. Mishra**
Resonance – Journal of Science Education (2025) In Press
96. Ultrasound-Assisted Polyphenol Hydrogelation: Mechanistic Insights into Self-Assembly, Antioxidant and Dual Antibacterial Action Against Gram-Positive and Gram-Negative Pathogens
P. Nandi, S. Parida, D. Das, S. Bose Dasgupta, **S. Mishra**, N. Sarkar
ACS Applied Bio Materials (2025) In Press
95. Bench-Stable Fe(III)-Bimetallic Photocatalyst for Controlled Polymerization of Acrylates via LMCT Excited State
S. Dolai, S. Karmakar, P. Das, **S. Mishra**, and S. K. Patra
Organometallics 44 (2025) 2481-2486
94. Blockwise Optimization for Projective Variational Quantum Dynamics (BLOP-VQD): Algorithm and Implementation for Lattice Systems
H. Singh, S. Majumder, and **S. Mishra**
J. Chem. Phys. 163 (2025) 124104
93. Redox-Assisted Controlled Radical Polymerization of Acrylates by Strategically Designed RuII-FeII Heterobimetallic Conjugate
S. Dolai, S. Karmakar, S. Kundu, **S. Mishra**, and S. K. Patra
Chem. Eur. J. (2025) e01951
92. Photoluminescence in Square Planar Ni(II) Complexes: A Study of Electronic Structure and Quantum Dynamics
K. K. Dakua, R. Sinha, and **S. Mishra**
Inorg. Chem. 64 (2025) 16323
91. Enhanced anodic charge storage in asymmetric hybrid supercapacitor featuring dione-diimide-based electron-deficient conjugated polymers

- D. Patra, S. K. Pati, S. Muduli, **S. Mishra**, G. Kim, and S. Park
J. Mat. Chem. A 13 (2025) 24694
90. Probing the Chemical Action of M–N₄ Motif in Metal Phthalocyanine-Based Redox Mediators in LiO₂ Batteries
S. Mandal, S. Parida, **S. Mishra**, and A. J. Bhattacharya
ChemSusChem (2025) e202501040
89. Energy Storage Behavior of Side Chain-Engineered Si-Bridged Redox-Active Donor-Acceptor Conjugated Polymers Operated in Organic Electrolyte
S. K. Pati, S. Muduli, D. Patra, S. Oh, B. Kim, **S. Mishra**, and S. Park
J. Mat. Chem. A 13 (2025) 20504
88. Hole and Electron Mobility in Sulfur- and BN-Functionalized Perylene Diimides: A Computational Study
S. Parida, S. K. Patra, and **S. Mishra**
J. Phys. Chem. C 129 (2025) 10264
87. Magnetostructural Correlation in Trigonal Bipyramidal Fe(III) Complexes: Tuning Spin-State Stability and Magnetic Anisotropy via Second Coordination Sphere Substitution
S. Joshi, S. Roy Chowdhury, and **S. Mishra**
Cryst. Growth Des. 25 (2025) 2602
86. Conformational Isomerization in Co(acac)₂ via Spin-State Switch: A Computational Study
S. Joshi, S. Roy Chowdhury, and **S. Mishra**
Dalton Trans. 54 (2025) 6081.
85. SHARC-VQE: Simplified Hamiltonian Approach with Refinement and Correction enabled Variational Quantum Eigensolver for Molecular Simulation
H. Singh, S. Majumder, and **S. Mishra**
J. Chem. Phys. 162 (2025) 114117
84. Modulating Enzyme's Conformational Space: Impact of Substrate Binding, Mode Alteration, and Active Site Mutation in DapC, an Aminotransferase Enzyme of Lysine Biosynthetic Pathway
S. Manna and **S. Mishra**
J. Phys. Chem. B 129 (2025) 2828
83. Flavin-Mediated Reductive Deiodination: Conformational Events and Reactivity Pattern in the Active Site of Human Iodotyrosine Deiodinase
S. Karmakar and **S. Mishra**
Biochemistry 63 (2024) 3310
82. Structure-Spectroscopy Correlation in the Self-assembled Perylene-diimide based dimers via Inter-Chromophore Coupling
S. Parida, S. K. Patra, and **S. Mishra**
J. Phys. Chem. B. 128 (2024) 9873
81. Ab Initio Calculation of Magnetic Anisotropy and Thermal Spin Transition in the Variable Temperature Crystal Conformations of [Co(terpy)₂]²⁺
M. Nath, S. Joshi, and **S. Mishra**
Phys. Chem. Chem. Phys. 26 (2024) 15405-15416.
80. Hückel Molecular Orbital Theory on a Quantum Computer: A Scalable System-Agnostic Variational Implementation with Compact Encoding
H. Singh, S. Majumder, and **S. Mishra**
J. Chem. Phys. 160 (2024) 194106.

79. Conformational Dynamics in *Corynebacterium glutamicum* Diaminopimelate Epimerase: Insights from Ligand Parametrization, Atomistic Simulation, and Markov State Modeling
S. Muduli, S. Karmakar, and **S. Mishra**
J. Chem. Inform. Model. 64 (2024) 4250-4262.
78. Heteroleptic Magnesium n-Butyl on a Chemically Non-innocent 2-Anilidomethylpyridine Ligand Leading to Diverse Magnesium Hydrides
C. Mandal, S. Joshi, **S. Mishra**, and D. Mukherjee
Inorg. Chem. 63 (2024) 15692
77. Conjugated Polymer Electrodes Fabricated Using Rylene-Based Acceptors Toward High Energy and Power Density Symmetric Supercapacitor Operable in Organic Electrolyte Environment
S. K. Pati, D. Patra, S. Muduli, **S. Mishra**, S. Park
J. Mat. Chem. A 12 (2024) 21165.
76. 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. 63 (2024) 4839.
75. 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.
74. 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.
73. 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.
72. 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.
71. 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.
70. 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.
69. 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.
68. 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.

67. 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.
66. 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.
65. 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.
64. 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
63. 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.
62. 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.
61. 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.
60. 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.
59. Identification of Potential Inhibitors Against FemX of Staphylococcus Aureus: A Hierarchical in-silico Drug Repurposing Approach
S. Rahman, K. Rajak, **S. Mishra**, and A. K. Das
J. Mol. Graph. Model. 115 (2022) 108215.
58. 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.
57. 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.

56. 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.
55. 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.
54. 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.
53. 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.
52. 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 π -interactions
V. K. Jha, S. Das, V. Subramaniyan, T. Guchhait, K. K. Dakua, **S. Mishra**, and G. Mani
Dalton Trans. 50 (2021) 8036-8044.
51. 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.
50. Flipped Regiospecificity in L434F Mutant of 8-Lipoxygenase
V. K. Mishra and **S. Mishra**.
Phys. Chem. Chem. Phys. 22 (2020) 16013-16032.
49. Correlation Effects in the Photoelectron Spectrum and Photoionization Dynamics of OsO₄
S. Manna and **S. Mishra**.
Phys. Chem. Chem. Phys. 22 (2020) 628-641.
48. 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.
47. Role of Substituents at 3-position of Thienylethynyl Spacer on Electronic Properties in Diruthenium(II) Organometallic Wire-like Complexes
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Chem. Asian J. 15 (2020) 3304-3313.
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