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

Research Supervision

- PhD Thesis Supervision: 4 awarded, 1 submitted, 5 SRF, 2 PMRF, 1 JRF.
- MSc Thesis Supervision: 14 completed; 3 in progress.

Teaching

Courses taught in 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)
- Quantum Methods in Molecular Simulations (TS62002/CD61006)

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).

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).

Presentation at Conferences/Symposia

- 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

- Convener/Organizer: 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. Ligands-Induced Open-Close Conformational Change during DapE Catalysis: Insights from Molecular Dynamics Simulations
   S. Muduli and **S. Mishra**
   Proteins: Struct. Funct. Bioinform. (2023) In press.
2. 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 (2023) In press.
3. 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. 2023 In press.
4. 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.
5. Electron Density in the Multiscale Treatment of Biomolecules,
   S. Karmakar, S. Muduli, A. Paul, and **S. Mishra**
   In Fundamentals of Electron Density. Nova Science Publishers, (2023) In press.
6. 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.
7. 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.
8. 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.
9. 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.
10. 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.

11. 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.
12. 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.
13. 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.
14. 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.
15. 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.
16. 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.
17. Flipped Regiospecificity in L434F Mutant of 8-Lipoxygenase
V. K. Mishra and **S. Mishra**.
Phys. Chem. Chem. Phys. 22 (2020) 16013-16032.
18. 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.
19. 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.
20. 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.
21. 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.
22. 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.

23. 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.
24. 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.
25. 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.
26. 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"
27. 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.
28. 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.
29. 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.
30. Ab Initio Investigation of Magnetic Anisotropy in Intermediate Spin Iron(III) Complexes.
S. Roy Chowdhury and **S. Mishra**.
J. Chem. Phys. 149 (2018) 234302.
31. Vibronic Structures and Photoelectron Angular Distribution in the Photoelectron Spectrum of ICN.
S. Manna and **S. Mishra**.
J. Chem. Phys. 149 (2018) 204308.
32. 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.
33. 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.
34. 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.

35. Synthesis, Structure, and Photophysical and Electrochemical Properties of Ru(II) Complexes of Arylenevinylene Terpyridyl Conjugates.
A. Sil, S. Roy Chowdhury, **S. Mishra**, and S. K. Patra.
Dalton Trans. 47 (2018) 9877-9888.
36. 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.
37. 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.
38. 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.
39. 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.
40. 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.
41. 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.
42. 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.
43. 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.
44. 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.
45. 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.

46. 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.
47. 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.
48. 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.
49. 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.

Before Joining IIT Kharagpur

50. Dynamics in the active site of β-secretase: A network analysis of atomistic simulations.
    S. Mishra and A. Caflisch. Biochemistry 50 (2011) 9328.
51. Quantitative analysis of ligand migration from transition networks.
    S. Mishra and M. Meuwly. Biophys. J. 99 (2010) 3969.
52. Atomistic simulation of NO dioxygenation in group I truncated hemoglobin.
    S. Mishra and M. Meuwly. J. Am. Chem. Soc. 132 (2010) 2968.
53. 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.
54. 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.
55. 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.
56. 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.
57. 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.
58. Theoretical calculation of photodetachment spectra of $XAuY^-$, (X, Y= Cl, Br, and I).

S. Mishra. J. Phys. Chem. A 111 (2007) 9164.

59. 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.
60. Quasistationary upper-well states of E×E Jahn-Teller systems with spin-orbit coupling.
L. V. Poluyanov, **S. Mishra**, and W. Domcke. Chem. Phys. 332 (2007) 243.
61. Quasiclassical calculation of the vibronic energy levels of the E×E Jahn-Teller effect including spin-orbit coupling.
L. V. Poluyanov, **S. Mishra**, and W. Domcke. Mol. Phys. 105 (2007) 1471.
62. 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.
63. 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.
64. 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.
65. 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.
66. The relativistic E×E Jahn-Teller effect revisited.
W. Domcke, **S. Mishra**, and L. V. Poluyanov. Chem. Phys. 322 (2006) 405.
67. 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.