



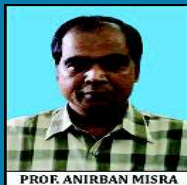
ENLIGHTENMENT TO EXCELLENCE

UNIVERSITY OF NORTH BENGAL

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Raja Ramohunpur, Dist- Darjeeling, West Bengal, Pin-734013, India.

Department of Chemistry

Print

**Dr. Anirban Misra**

M.Sc., M.Tech., Ph.D.

Professor

Life Member- Chemical Research Society of India; American Chemical Society (Honorary 3 years Membership),

Contact Addresses:

Contact No.	+919434228745(M)
Mailing Address	Department of Chemistry, University of North Bengal, P.O.- NBU, Dist- Darjeeling, West Bengal, Pin -734013, India.
e-Mail	anirbanmisra@yahoo.com ; anirbanmisra@nbu.ac.in

Subject Specialization: Physical Chemistry**Area of Specialization:** Theoretical Chemistry/ Quantum Chemistry / Computational Chemistry**No. of Ph.D. Students:** (a) Supervised: 8 (b) Ongoing: 5**No. of Publication:** (a) Journal Article: 73 (b) Book/Book Chapter: 01**Awards and Fellowships and Memberships:**

- Life Member CRSI
- Three year membership of ACS (Honorary)
- Visiting Scientific Fellow at Texas A & M University at Galveston in 2006.
- IBM-Lowdin Award at Sanibel 2003.
- Welch Post Doctoral Fellow in Texas A&M University at Galveston, Texas 2001- 2003.
- Chemical Research Society of India Research Award 2016.
- Chemical Research Society of India Bronze Medal 2018.

Post Doctoral Research: August, 2001 – May, 2003 at Texas A&M University at Galveston, Texas**Professional Experience:**

- 21 Years in Academics and 3 years in Industry

Research Area:

- Theoretical Investigation on Magnetism and Magnetic Molecules
- Aromaticity
- Quantum Chemistry
- Chemical Graph Theory
- Spin wave theory
- Investigation of Optical and transport properties of molecules and materials.

Research Projects:

- Completed: DST Project “Development of Relativistic Theories of Magnetism in Atoms and Molecules and Investigation of Magnetism in High-spin Systems”
- Completed: DST Project “Theoretical investigation of nanomagnetic systems and their possible applications as spintronic materials”
- Completed: CSIR Project “Theoretical Investigation of Aromatic Systems and Search for New Quantum Chemical Descriptor of Aromaticity”
- (Completed: SERB-DST Project: “Theoretical Investigation of Optical, Transport and Magnetic Properties in Mesoscopic Systems”

Teaching:**Present Courses:**

- Quantum Mechanics (For M.Sc. First Year Students)
- Quantum Chemistry I (For M.Sc. First Year Students)
- Quantum Chemistry II (For Physical Chemistry Special Students)
- Nonequilibrium Thermodynamics (For Physical Chemistry Special Students)
- Quantum Chemistry Lab (For Physical Chemistry Special Students)
- Advanced Quantum Chemistry (For Ph.D. Students)

List of Publications:

- M. Homray, S. Mondal, A. Misra and P. K. Chattaraj, Bond stretch isomerism in Be₃ 2- driven by the Renner–Teller effect, *Phys. Chem. Chem. Phys.* DOI: 10.1039/c9cp00643e (2019).
- T. Sutradhar and A. Misra, Enhancement of Nonlinear Optical Properties of Indole Based Dyes through Electron Acceptor and π -Linker for Dye-Sensitized Solar Cell Applications, *ChemistrySelect*, **4**, 3697-3705 (2019).
- M. Homray, S. Paul and A. Misra, Manifestation of exo-cyclic aromaticity in triangular heterocyclic B₂F₂X Systems (X=O, S, Se, NH), *Bull. Mater. Sci.* **42**:46 (2019).
- M. Majumder, S. Paul, and A. Misra Ligand Induced Symmetry Breaking and Concomitant Blue Shift of Emission Wavelength in Octahedral Chromium Complex, *J. Mol. Model.* **24**, 230-8 (2018).
- M. Majumder and A. Misra, Strategic design of thiophene-fused nickel dithiolene derivatives for efficient NLO response, *Phys. Chem. Chem. Phys.* **20**, 9364-9375 (2018).
- T. Sutradhar and A. Misra, Role of Electron-Donating and Electron-Withdrawing Groups in Tuning the Optoelectronic Properties of Difluoroboron–Naphthyridine Analogues, *J. Phys. Chem. A*, **122**, 4111–4120 (2018).
- P. Sarbadhikary, S. Shil and A. Misra, Magnetic and Transport Properties of Conjugated and Cumulated Molecules: the π -System Enlightens Part of the Story, *Phys. Chem. Chem. Phys.* **20**, 9364-9375 (2018).
- M. Majumder, T. Goswami and A. Misra, Multifunctional Magnetic Materials of Organic Origin for Biomedical Applications: A Theoretical Study, *ChemistrySelect*, **3**, 933-939 (2018).
- S. Mandal, T. Goswami, G. H. Jana, A. Misra and P. K. Chattaraj, A possible reason behind the initial formation of pentagonal dodecahedron cavities in sI-methane hydrate nucleation: A DFT study, *Chem. Phys. Lett.* **619**, 415-420 (2018).
- R. Kar, B. C. Paul and A. Misra, Unconventional superconductivity in iron pnictides: Magnon-mediated pairing, *Physica C*, **545**, 18-25 (2018).
- A. K. Mondal, T. Goswami, A. Misra and S. Konar, Probing the Effects of Ligand Field and Coordination Geometry on Magnetic Anisotropy of Pentacoordinate Cobalt(II) Single-Ion Magnets, *Inorg. Chem.* **56**, 6870–6878 (2017).
- T. Goswami, M. Homray, S. Paul, D. Bhattacharya and A. Misra, On Exo-cyclic Aromaticity, *Phys. Chem. Chem. Phys.* (Communication) **19**, 11744-11747 (2017).
- S. Sarkar, T. Goswami, D. Bhattacharya and A. Misra, On the performance of generalized valence bond theory in predicting magnetic exchange coupling constant in organic diradicals: A comparison with Hartree-Fock theory, *comp. theor. Chem.*, **1116**, 220 (2017).
- M. Homray, A. Misra and P. K. Chattaraj, Aromaticity in the light of magnetic criterion, *Curr. Org. Chem.* **21**, 2699-2704 (2017).
- D. Bhattacharya, S. Shil, A. Misra, L. Bytautas and D. J. Klein, Toward Molecular Magnets of Organic Origin via Anion– π Interaction Involving m-Aminyl Diradical: A Theoretical Study, *J. Phys. Chem. A*, **120**, 9117–9130 (2016).
- S. Shil, P. Sarbadhikary and A. Misra, Effect of length on the transport and magnetic properties of diradical substituted molecular wires, *RSC Adv.* **6**, 99467-99474 (2016).
- P. Sarbadhikary, S. Shil, A. Panda and A. Misra, A Perspective on Designing Chiral Organic Magnetic Molecules with Unusual Behavior in Magnetic Exchange Coupling, *J. Org. Chem.* **81**, 2623-2630 (2016).
- S. Shil, M. Roy and A. Misra, Role of Coupler to Design Organic Magnetic Molecules: LUMO Plays an Important Role in Magnetic Exchange, *RSC Adv.* **5**, 105574 – 105582 (2015).
- [S. Sarkar](#), [P. Ghosh](#), [A. Misra](#) and [S. Das](#), [Regio-Controlled Nitration of 4-Quinolones at Ambient Conditions](#), *Synth. Commun.* **45**, 2386-2393 (2015).
- S. Pal, T. Goswami and A. Misra, Noncomparative scaling of aromaticity through electron itinerancy, *AIP Adv.* **5**, 107211 (2015).
- S. Shil, D. Bhattacharya, A. Misra and D. J. Klein, A high-spin organic diradical as a spin filter, *Phys. Chem. Chem. Phys.* **17**, 23378 (2015).
- D. Bhattacharya, S. Shil, A. Misra, L. Bytautas and D. J. Klein, Photomagnetic and Nonlinear Optical Properties in cis-trans Green Fluoroprotein Chromophore Coupled Bis-Imino Nitroxide Diradicals, *Int. J. Quantum Chem.* **115**, 426-433 (2015).

- D. Bhattacharya, S. Shil, A. Misra, L. Bytautas and D. J. Klein, Borazine: spin blocker or not?, *Phys. Chem. Chem. Phys.* **17**, 14223-14237 (2015).
- T. Goswami, S. Paul, S. Mandal, A. Misra, A. Anoop and P. K. Chattaraj, On the Existence of Bond Stretch Isomerism in Be_3^{2-} : A Theoretical Account, *Int. J. Quantum Chem.* **115**, 426-433 (2015).
- R. Kar, T. Goswami, B.C. Paul and A. Misra, On magnon mediated Cooper pair formation in ferromagnetic superconductors, *AIP Adv.* **4**, 087126-12 (2014).
- T. Goswami and A. Misra, On the Control of Magnetic Anisotropy through External Electric Field, *Chem. Euro. J.* **20**, 13951 – 13956 (2014).
- D. Bhattacharya, A. Panda, A. Misra and D. J. Klein, Clar Theory Extended for Polyacenes and Beyond, *J. Phys. Chem. A.* **118**, 4325–4338 (2014).
- D. Bhattacharya, S. Shil, T. Goswami, A. Misra and D. J. Klein, A note on second-order nonlinear optical response of high-spin bis-TEMPO diradicals with possible application, *Comput. Theor. Chem.* **1039**, 11-14 (2014).
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- S. Sarkar, S. Shil and A. Misra, DFT based study on the mechanism of an unexpected reaction of aldehydes with 1,3-dicarbonyl compounds, *J. Ind. Chem. Soc. A* (Accepted 2014). **91**, 1289-1297 (2014).
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Book Chapter:

- "Diradical Based Organic Molecular Magnetism: Theory and Applications" Debojit Bhattacharya, Anirban Panda, Anirban Misra, (Nova Publishers, 2011).