C.V.

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3. Academic qualifications:

Degree	University
M.Sc.	I.I.T. Kharagpur
M. Tech.	I.I.T. Bombay
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Post Doctoral Research	Texas A & M University at Galveston

4. Awards and Fellowships and Memberships:

Life Member CRSI
Visiting Scientific Fellow at Texas A & M University at Galveston in 2006.
IBM-Lowdin Award at Sanibel 2003.

5. Research Area: Theoretical Chemistry, Quantum Chemistry

6. Total Number of Publications: Journal Papers 48, Book Chapter 1

7. Number of Ph.D. Produced: Completed 2, Thesis submitted 2, On Going 4.

8. <u>List of Publications (Since 2009)</u>:

1. T. Goswami and A. Misra, On the Control of Magnetic Anisotropy through External Electric Field, *Chem. Euro. J.* (Provisionally Accepted 2014).
2. D. Bhattacharya, A. Panda, A. Misra and D. J. Klein, Clar Theory Extended for Polyacenes and Beyond, *J. Phys. Chem. A.* (Accepted 2014).
3. 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).
4. T. Goswami, S. Paul and A. Misra, Effect of Charge Transfer and Periodicity on the Magnetism of $[Cr(Cp^*)_2][ETCE]$, *RSC Adv.* **4**, 14847-14857 (2014).
5. 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).
6. B. Sinha, T. Goswami, S. Paul and A. Misra, The impact of surface structure and band gap on the optoelectronic properties of Cu_2O nanoclusters of varying size and symmetry, *RSC Adv.* **4**, 5092–5104 (2014).
7. D. Bhattacharya, S. Shil, T. Goswami, A. Misra, A. Panda and D.J. Klein, A Theoretical Study on Magnetic Properties of Bis-TEMPO Diradicals with Possible Application, *Comput. Theor. Chem.* **1024**, 15-23 (2013).
8. M. Majumder, T. Goswami, A. Misra, S. Bardhan and S. K. Saha, Intermolecular Interaction in 2-Aminopyridine: A Density Functional Study, *Commun. Comput. Chem.* **1**, 225-243 (2013).
9. S. Paul, T. Goswami, A. Misra and P. K. Chattaraj, Concurrent loss of aromaticity and onset of superexchange in Mg_3Na_2 with an increasing Na – Mg_3 distance, *Theor. Chem. Acc.* **132**, 1391-10 (2013).
10. S. Shil and A.Misra, Electric Field Induced Tuning of Molecular Conformation to Acquire Spintronics Property in Biphenyl Systems, *RSC Adv.* **3**, 14352-14362 (2013).

11. S. Shil, D. Bhattacharya, S. Sarkar and A. Misra, Performance of the Widely Used Minnesota Density Functionals for the Prediction of Heat of Formations, Ionization Potentials of Some Benchmarked First Row Transition Metal Complexes, *J. Phys. Chem. A.* **117**, 4945-4955 (2013).
12. S. Shil, S. Paul and A. Misra, Charge Transfer Induced Magnetism in Mixed-stack Complexes, *J. Phys. Chem. C*, **117**, 2016-2023 (2013).
13. T. Goswami and A. Misra, Ligand Effects toward the Modulation of Magnetic Anisotropy and Design of Magnetic Systems with Desired Anisotropy Characteristics, *J. Phys. Chem. A.* **116**, 5207-5215 (2012)**.**
14. R. Kar, A. Misra, N. H. March and D. J. Klein, Bose-Einstein Condensation of Magnons in Ferromagnetic Thin Films, *Phase Transitions*, **85**, 831-839 (2012).
15. D. Bhattacharya, A. Panda, S. Shil, T. Goswami and A. Misra, A Theoretical Study on Photomagnetic Fluorescent Protein Chromophore Coupled Diradicals and Their Possible Applications, *Phys. Chem. Chem. Phys.* **14**, 6509-6913 (2012).
16. S. Paul and A. Misra, Interpretation and quantification of magnetic interaction through spin topology, *J. Chem. Theory Comput.* **8**, 843-853 (2012).
17. S. Paul and A. Misra, Interplay among aromaticity, magnetism and nonlinear optical response in all-metal aromatic systems, *Inorg. Chem.* **50**, 3234-3246 (2011).
18. A. Misra and A. Panda, On the Variation of Ortho-hydrogen and Para-hydrogen Ratio with Magnetic Field Strength at Low Temperature, *J. Low Temp. Phys.* **163**, 311-316 (2011).
19. D. Bhattacharya, S. Shil and A. Misra, Photoresponsive Magnetization Reversal in Green Fluorescent Protein Chromophore Based Diradicals, *J. Photochem. Photobiol. A: Chem.* **217**, 402-410 (2011).
20. D. Bhattacharya, S. Shil, A. Panda and A. Misra, A DFT study on the magneto-structural property of ferromagnetic heteroverdazyl diradicals with phenylene coupler, *J. Phys. Chem. A.* **114**, 11833-11841 (2010).
21. R. Kar and A. Misra, Rise of temperature in ferromagnetic nanoparticles due to perpendicular pumping, *Nanosci. Nanotechnol. Lett.* **2**, 253-256 (2010).
22. S. Paul and A. Misra, Exchange interactions in systems with multiple magnetic sites, *J. Phys. Chem. A.* **114**, 6641-6647 (2010).

23. S. Shil and A. Misra, Photoinduced antiferromagnetic to ferromagnetic crossover in organic systems, *J. Phys. Chem. A.* **114**, 2022-2027 (2010).
24. D. Bhattacharya, S. Shil, A. Misra and D. J. Klein, Intramolecular ferromagnetic coupling in bis-oxoverdazyl and bis-thioxoverdazyl diradicals with polyacene spacers, *Theor. Chem. Acc.* **127**, 57-67 (2010).
25. R. Kar and A. Misra, Increase in temperature of a ferromagnetic substance in rf magnetic field, *J. Magn. Magn. Mater.* **322**, 671-674 (2010).
26. A. Misra, T. G. Schmalz and D. J. Klein, Clar theory for radical benzenoids, *J. Chem. Inf. Model.* **49**, 2670-2676 (2009).
27. S. Sarkar, S. Shil, S. Paul and A, Misra, On protonationa and methylation of benzene: a B3LYP DFT based study, *J. Mol. Struct. (THEOCHEM)* **916**, 154-158 (2009).
28. D. Bhattacharya and A. Misra, Density functional theory based study of magnetic interactions in bis-oxoverdazyl diradicals connected by different aromatic couplers, *J. Phys. Chem. A.* **113**, 5470-5475 (2009).
29. S. Paul and A. Misra, On magnetic nature of Mn clusters, *J. Mol. Struct. (THEOCHEM)* **907**, 35-40 (2009).
30. A. Misra, D. J. Klein and T. Morikawa, Clar theory on molecular benzenoids, *J. Phys. Chem A.***113**, 1151–1158 (2009).
31. S. Paul and A. Misra, Magnetic properties of $Cr_2O_n^-$ clusters: a theoretical study, *J. Mol. Struct. (THEOCHEM)* **895** 156-160 (2009).