

Previous Publications (Prior to Joining IIT Mandi)

40. **B. Mondal**, S. Ye, Hidden Ligand Noninnocence: A Combined Spectroscopic and Computational Perspective, *Coord. Chem. Rev.* 405, 213115, 2020.
‡Special Issue dedicated to Prof. G. K. Lahiri's 60th Birthday
39. S. Agasti, **B. Mondal**, T. K. Achar, S. K. Sinha, A. S. Suseelan, K. J. Szabo, F. Schoenebeck, D. Maiti, Orthogonal Selectivity in C–H Olefination: Synthesis of Branched Vinylarene with Unactivated Aliphatic Substitution, *ACS Catal.*, 9, 9606–9613, 2019.
38. H-C. Chang[‡], **B. Mondal**[‡], H. Fang, F. Neese, E. Bill*, S. Ye* EPR Signature of Tetragonal Low Spin Iron(V)-Nitrido and -Oxo Complexes Derived from the Electronic Structure Analysis of Heme and Non-Heme Archetypes, *J. Am. Chem. Soc.*, 141, 2421-2434, 2019.
‡Joint First Author
37. L. Roy, M. H. Al-Afyouni, D. E. DeRoshia, **B. Mondal**, I. M. DiMucci, K. M. Lancaster, J. Shearer, E. Bill, W. W. Brennessel, F. Neese, S. Ye, P. L. Holland, Mechanism of Reduction of CO₂ by a Masked Two-Coordinate Cobalt(I) Complex Through an Isolable Oxodicobalt(II) Species, *Chem. Sci.*, 10, 918-929, 2019.
36. **Mondal, B.**; Neese, F.; Ye, S. "Computational Insights into Chemical Reactivity and Road to Catalyst Design: The Paradigm of CO₂ Hydrogenation" in Non-Noble Metal Catalysis: Molecular Approaches and Reactions, Eds. Gebbink, R. J. M. K.; Moret, M-E, *Wiley VCH*, 2018, pp. 33-48)*
‡Invited Book Chapter
35. **B. Mondal**, F. Neese, E. Bill, S. Ye, Electronic Structure Contributions of Non-Heme Oxo-Iron(V) Complexes to the Reactivity, *J. Am. Chem. Soc.*, 140, 9531-9544, 2018.
34. C. Kupper[‡], **B. Mondal**[‡], J. Serrano-Plana, I. Klawitter, F. Neese, M. Costas, S. Ye, F. Meyer, Non-Classical Single-State Reactivity of an Oxo-Iron(IV) Complex Confined to Triplet Pathways, *J. Am. Chem. Soc.*, 139, 8939-8949, 2017.
‡Joint First Author
33. S. Ye, C. Kupper, S. Meyer, E. Andris, R. Navrátil, O. Krahe, **B. Mondal**, M. Atanasov, E. Bill, J. Roithová, F. Meyer, F. Neese, Magnetic Circular Dichroism Evidence for an Unusual Electronic Structure of a Tetracarbene-Oxoiron(IV) Complex, *J. Am. Chem. Soc.*, 138, 14312-14325, 2016.
32. **B. Mondal**, L. Roy, F. Neese, S. Ye, High-Valent Iron-Oxo and -Nitrido Complexes: Bonding and Reactivity, *Isr. J. Chem.*, 56, 763-772, 2016.
‡In honor of Professor Harry B. Gray's career
31. **B. Mondal**, F. Neese, S. Ye, Toward Rational Design of 3d Transition Metal Catalysts for CO₂ Hydrogenation Based on Insights into Hydricity-Controlled Rate-Determining Steps, *Inorg. Chem.*, 55, 5438-5444, 2016.
30. **B. Mondal**, F. Neese, S. Ye, Control in the Rate-Determining Step Provides a Promising Strategy To Develop New Catalysts for CO₂ Hydrogenation: A Local Pair Natural Orbital Coupled Cluster Theory Study, *Inorg. Chem.*, 54, 7192-7198, 2015.
29. **B. Mondal**, J. Song, F. Neese, S. Ye, Bio-inspired mechanistic insights into CO₂ reduction, *Curr. Op. Chem. Biol.*, 25, 103-109, 2015.

28. J. A. Brown, A. R. Cochrane, S. Irvine, W. J. Kerr, **B. Mondal**, J. A. Parkinson, L. C. Paterson, M. Reid, T. Tuttle, S. Andersson, G. N. Nilsson, The Synthesis of Highly Active Iridium(I) Complexes and their Application in Catalytic Hydrogen Isotope Exchange, **Adv. Synth. Catal.**, 356, 3551-3562, 2014.
‡Inside Cover
27. A. R. Cochrane, C. Idziak, W. J. Kerr, **B. Mondal**, L. C. Paterson, T. Tuttle, S. Andersson, G. N. Nilsson, Practically convenient and industrially-aligned methods for iridium-catalysed hydrogen isotope exchange processes, **Org. Biomol. Chem.**, 12, 3598-3603, 2014.
26. **B. Mondal**, R. D. Wilkes, J. M. Percy, T. Tuttle, R. J. G. Black, C. North, Towards a quantitative understanding of palladium metal scavenger performance: an electronic structure calculation approach, **Dalton Trans.**, 43, 469-478, 2014.
25. S. Zhou, G. M. Anderson, **B. Mondal**, E. Doni, V. Ironmonger, M. Kranz, T. Tuttle, J. A. Murphy, Organic super-electron-donors: initiators in transition metal-free haloarene-arene coupling, **Chem. Sci.**, 5, 476-482, 2014.
‡Cover Article
24. C. Sahu, K. Sen, S. Pakhira, **B. Mondal**, A. K. Das, Binding affinity of substituted ureido-benzenesulfonamide ligands to the carbonic anhydrase receptor: A theoretical study of enzyme inhibition, **J. Comput. Chem.**, 34, 1907-1916, 2013.
23. K. Sen, **B. Mondal**, S. Pakhira, C. Sahu, D. Ghosh, A. K. Das, Association reaction between SiH₃ and H₂O₂: a computational study of the reaction mechanism and kinetics. **Theor. Chem. Acc.**, 132, 1375-1391, 2013.
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21. S. Pakhira, D. Mandal, **B. Mondal**, A. K. Das, Theoretical study of spectroscopy, interaction, and dissociation of linear and T-shaped isomers of RgClF (Rg = He, Ne, and Ar) van der Waals complexes, **Struct. Chem.**, 23, 681-692, 2012.
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19. **B. Mondal**, D. Mandal, A. K. Das, Pyrolysis of *tert*-Butyl *tert*-Butanethiosulfinate, *t*-BuS(O)St-Bu: A Computational Perspective of the Decomposition Pathways, **J. Phys. Chem. A**, 115, 3068-3078, 2011.
18. S. Pakhira, **B. Mondal**, A. K. Das, Spectroscopic properties of I₂-Rg (Rg = He, Ne, Ar) van der Waals complexes, **Chem. Phys. Lett.**, 505, 81-86, 2011.
17. S. Bagchi, I. Bhattacharyya, **B. Mondal**, A. K. Das, Structure, stability and energetics of ionic arsenic-water complexes. **Mol. Phys.**, 109, 933-941, 2011.
16. **B. Mondal**, D. Ghosh, A. K. Das, Theoretical study of [Si, O, C, O] species: Prediction of new species on triplet potential energy surface, **Int. J. Quantum Chem.**, 111, 606-615, 2011.

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14. D. Ghosh, **B. Mondal**, S. Bagchi, A. K. Das, Isomers of OCS and their reaction with H₂O on singlet potential energy surface, *Mol. Phys.*, 108, 3353-3364, 2010.
13. D. Mandal, **B. Mondal**, A. K. Das, Isomerization and Decomposition of a Model Nerve Agent: A Computational Analysis of the Reaction Energetics and Kinetics of Dimethyl Ethylphosphonate, *J. Phys. Chem. A*, 114, 10717-10725, 2010.
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9. **B. Mondal**, D. Mandal, D. Ghosh, A. K. Das, Computational Study on the Growth of Gallium Nitride and a Possible Source of Oxygen Impurity, *J. Phys. Chem. A*, 114, 5016-5025, 2010.
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1. **B. Mondal**, N. C. Bera, A. K. Das, Stability, spectroscopic constants, and dissociation of CO²⁺: A theoretical study, *Int. J. Quantum Chem.*, 109, 469-476, 2009.