

Publications from Supervised Research (PhD and PostDoc)

Dr. Bhaskar Mondal

43. M. Mendel, T. M. Karl, J. Hamm, S. J. Kaldas, T. Sperger, **B. Mondal**, F. Schoenebeck, Dynamic stereomutation of vinylcyclopropanes with metalloradicals, *Nature*, 2024, <https://doi.org/10.1038/s41586-024-07555-1>.
42. L. Roy[‡], **B. Mondal**[‡], S. Ye, Computational mechanistic insights into non-noble-metal-catalysed CO₂ conversion, *Dalton Trans.*, 49, 16608-16616, 2020.
‡Equal Contribution
41. L. Roy, **B. Mondal**, F. Neese, S. Ye, “Theoretical Approach to Homogeneous Catalytic Reduction of CO₂: Mechanistic Understanding to Build New Catalysts” in Carbon Dioxide Electrochemistry: Homogeneous and Heterogeneous Catalysis, Chapter 5, Eds. M. Robert, C. Costentin, K. Daasbjerg, *Royal Society of Chemistry*, 2020.
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.
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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*, pp. 33-48 2018.
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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.
‡Equal Contribution
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,

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‡In honor of Professor Harry B. Gray's career
32. **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.
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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.
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