List of publications:

1. Tuning the Type 1 Reduction Potential of Multicopper Oxidases: Uncoupling the Effects of Electrostatics and H-Bonding to Histidine Ligands
   Asmita Singha, Alina Sekretareva, Lizhi Tao, Hyeongtaek Lim, Yang Ha, Augustin Braun, Stephen M. Jones, Britt Hedman,§ Keith O. Hodgson, R. David Britt, Daniel J. Kosman*, Edward I. Solomon*
   J. Am. Chem. Soc., **2023**, *145*, 24, 13284−13301
   [https://doi.org/10.1021/jacs.3c03241]

2. Oxygen Reduction by Iron Porphyrins with Covalently Attached Pendent Phenol and Quinol.
   Asmita Singha, Arnab Mondal, Abhijit Nayek, Somdatta Ghosh Dey, and Abhishek Dey*
   J. Am. Chem. Soc., **2020**, *142*, 52 21810−21828
   [https://doi.org/10.1021/jacs.0c10385]

3. Resonance Raman Spectroscopy and Density Functional Theory Calculations on Ferrous Porphyrin Dioxygen Adducts with Different Axial Ligands: Correlation of Ground State Wave Function and Geometric Parameters with Experimental Vibrational Frequencies
   Asmita Singha, Pradip Kumar Das, and Abhishek Dey*
   Inorg. Chem., **2019**, *58*, 16, 10704−10715
   [https://doi.org/10.1021/acs.inorgchem.9b00656]

4. Mechanism of Reduction of Ferric Porphyrins by Sulfide: Identification of a Low Spin $Fe^{III}-SH$ Intermediate
   Kaustuv Mittra,[#] **Asmita Singha,[#]** and Abhishek Dey*
   # Both the authors contributed equally.
   Inorg. Chem., **2017**, *56*, 7, 3916 − 3925
   [https://doi.org/10.1021/acs.inorgchem.6b02878]

5. Hydrogen atom abstraction by synthetic heme ferric superoxide and hydroperoxide species
   Asmita Singha and Abhishek Dey*
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6. Effect of hydrogen bonding on innocent and noninnocent axial ligands bound to iron porphyrins
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   [https://doi.org/10.1039/C8DT03852J]

7. Nitrogen hybridization controls peroxo-oxo equilibrium in ethylenediamine bound binuclear $[Cu_2O_2]$ complexes
   Asmita Singha, Atanu Rana, Abhishek Dey*
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8. Second sphere control of spin state: Differential tuning of axial ligand bonds in ferric porphyrin complexes by hydrogen bonding
   Kaustuv Mittra, Kushal Sengupta, **Asmita Singha**, Sabyasachi Bandyopadhyay, Sudipta Chatterjee, Atanu Rana, Subhra Samanta, Abhishek Dey*
   Journal of Inorganic Biochemistry, **2016**, *155*, 82–91
   [https://doi.org/10.1016/j.jinorgbio.2015.11.013]

9. Iron porphyrins with a hydrogen bonding cavity: effect of weak interactions on their electronic structure and reactivity
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   Dalton Trans., **2016**, *45*, 18796-18802
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10. Synthetic heme dioxygen adducts: electronic structure and reactivity
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    Dr. Azaj Ansari, Mursaleem Ansari, **Asmita Singha**, Prof. Gopalan Rajaraman*
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    Kaustuv Mittra, Subhra Samanta, **Asmita Singha**, Kushal Sengupta, Sudipta Chatterjee
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