COMPUTATIONAL INSIGHTS IN EXPLORING LIGAND AND SOLVENT EFFECTS ON THE REACTIVITY OF NON-HEME IRON-OXO BIO-MIMETIC CATALYSIS

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Non-heme iron-oxo bio-mimetic catalysts have emerged as promising bio-inspired candidates for various reactions, including oxidation, hydroxylation (specifically hydrogen atom transfer or HAT), and epoxidation. Besides the experiment, computational studies have become recently a vital tool in designing and optimizing such catalysts. It has been shown that the reactivity of non-heme iron-oxo bio-mimetic catalysts is strongly dependent on the electronic structure of the iron centre, which can be tuned by modifying the ligands. Additionally, solvent effects may significantly impact the reaction rate and selectivity of these catalysts [1,2]. Detailed information on the reactivity of such bio-mimetic complexes is required for the development of more efficient and sustainable catalysts for industrial and environmental applications. In this work, we present our computational results on the investigation of the electronic structure and reaction mechanisms of three non-heme iron-oxo bio-mimetic catalysts. To do so, we use different computational approaches, including *ab initio* single- and multireference methods (e.g., LUCCSD(T), DLPNO-CCSD(T), PNO-CCSD(T), and CASPT2) to explore the catalytic activity of these systems and to elucidate the role of the ligands and solvent on their reactivity.

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[2] Q. M. Phung, C. Martín-Fernández, J. N. Harvey, and M. Feldt, Ab Initio Calculations for Spin-Gaps of Non-Heme Iron Complexes, *J. Chem. Theory Comput.*, **2019**, *15 (8)*, 4297-4304.