Biocatalysts and Synthetic Catalysts: A Needed Partnership between Quantum and Statistical Mechanics

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Computational modeling of catalytic systems requires an accurate description of molecular interactions and the ability to capture statistical fluctuations that is important for function. I will contrast what we know about biocatalysts, and how they could be used as a unifying descriptor for catalytic design across a range of homogeneous and heterogeneous synthetic catalysts including synthetic enzymes, supramolecular capsules, electrocatalysts and microdroplet chemistry. I will also discuss recent our methodological advances from accurate many-body force fields under non-reactive approximations to reactive force fields to describe chemical reactions where charge flow is an essential process.