Density Functional Theory QM/MM Studies of Mononuclear Non-heme Iron(II) Enzymes

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Theoretical calculations have been carried out to characterize reaction mechanisms of two mononuclear non-heme iron(II) enzymes: peptide deformylase and taurine/α-ketoglutarate dioxygenase. The former represents a novel class of mononuclear iron peptidase, while α-ketoglutarate dioxygenases constitute the largest known family of mononuclear non-heme iron-containing enzymes that play key roles in biosynthesis, oxygen sensing in cells , DNA/RNA repair and many metabolic pathways. Our computational approaches center on the combined density functional theory QM/MM method, which allows for accurate modeling of the chemistry at the metal active site while properly including the effects of protein environment.