

QM/MM analysis of metalloenzymes: developments and applications

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Abstract

In this talk I'll discuss our studies of metalloenzymes using QM/MM simulations, including both DFTB3/MM free energy simulations and strategies to improve the results with higher level QM/MM energetics. I'll also touch upon several other technical issues such as the effect of QM region size and the degree of conformational sampling required for a meaningful mechanistic analysis; these will be illustrated with specific examples such as Catechol O-methyltransferase and Human U six biogenesis protein 1 (USB1). I'll then discuss our latest results regarding the mechanism of DNA polymerase and the potential role of the third Magnesium ion in catalysis.