

P006 Metalloprotein Simulations: Who's Afraid of the Big Bad Transition Metal?

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Transition Metals (TMs) play key roles in many biological processes. However, since many TM centres are electronically complex, their treatment theoretically appears to require quantum mechanics (QM). QM is too expensive for the entire system prompting many to use hybrid QM/MM schemes while others shy away altogether from anything containing TMs. QM/MM codes are popular but they are limited by the relatively slow QM part and dynamics is prohibitively expensive. In contrast, classical Molecular Dynamics (MM) is much faster but current MD programs do not treat the important d electron effects which have significant structural and energetic consequences. In contrast, these effects can be accurately captured using empirical ligand field theory (LFT). Thus, a solution to the QM/MM problem is to replace the expensive QM part with cheap, parametrical LFT - Ligand Field Molecular Mechanics (LFMM). The advantages of LFMM are: (a) TMs are on the same footing as all other atoms in the force field (b) there is a uniform treatment of the entire system without the artificial quantum/classical boundary inherent in QM/MM (c) we can get the same answer as QM/MM orders of magnitude faster (d) MD simulations are feasible with fairly modest computational facilities. The utility and diversity of LFMM will be illustrated using simple coordination complexes and the oxidised T1 centres of blue copper proteins.