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Density functional theory applied to iron electron transfer systems

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Electron transfer can be thought of as the simplest chemical reaction; a single electron moves, via tunneling or hopping, from one molecular species to another. However, the cascade of events which follows that electron transfer is not so simple, and the physical properties of the electron donor, acceptor and surrounding molecules can change quite dramatically across both quantum and classical mechanical dimensions of space and time. This complexity makes electron transfer reactions good candidates for theoretical investigation. The process of electron transfer is essential to living things as manifested in cellular respiration and photosynthesis. Inter- and intra-molecular electron transfer reactions in biological systems are good prototypes for density functional methods (DFT), which have highly desirable features such as good parallel scalability, which makes such large quantum mechanical calculations possible, and electron correlation, which is crucial to accurately model energetic properties of metallic systems. DFT's positive and negative aspects will be discussed in the context of theoretical studies which model such properties as reduction potentials and electron hopping probabilities in iron metalloenzymes and smaller model systems.