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Bridging the gap between theoretical and experimentally inferred reorganization energy

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Biological electron transfer (ET) reactions are fundamental to the production of energy in all living cells. Efficient, site-selective electron transfer is crucial for effective metabolic processes to sustain life. An accurate description of the electron transfer process through a protein complex is lacking. In particular, with the MADH and amicyanin protein complex, found in the bacteria *Paracoccus denitrificans*, there is a disagreement between the theoretical prediction and the experimentally inferred reorganization energy. The reorganization energy is a poorly understood yet key element in describing qualitatively electron transfer though a metabolic protein complex. Attempts at better understanding the energetics of the reaction involve adapting Marcus thoery, the wildly successful model for simple electron transfer reactions yet problematic for complex systems. Previous work suggest a new model which includes electrostatic interactions between the protein complex and surrounding solvent in to the reorganization energy. In this theoretical work, we investigate the validity of the new model for ET in the MADH-amicyanin protein pair. The MADH-amicyanin system is chosen in part for its particular use of water in the active site of the reaction. We perform classical molecular dynamic simulations of the solvated protein pair. A set of trajectory steps/frames from the simulations are then analyzed using the combined quantum mechanical and molecular mechanical (QM/MM) scheme to calculate interaction energies. The molecular simulations performed in this investigation further support the importance of the solvent's role in the ET process. Furthermore, we provide evidence that the discrepancy between the theoretical and the experimentally inferred values of the reorganization energy can be minimized by including the protein-solvent interactions in the model.

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