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DFT Studies of the Quinone Electron Acceptor of Photosystem II and Related Model Systems[1] ELIJAH GRUSZECKI, AMANDA MANALTI, DAN XIAO, JEAN J. BENOIT, AMGALABAATAR BALDANSUREN, K. V. LAKSHMI, Rensselaer Polytechnic Institute — In photosynthetic and respiratory protein complexes, quinone cofactors participate in both proton and electron transfer. In Photosystem I (PSI), phylloquinones function to transfer electrons through the electron transport chain. In Photosystem II (PSII) and the bacterial reaction center, benzoquinones are used to facilitate both electron and proton coupled electron transfer (PCET). Previous experimental studies determined the redox potentials, solvent interactions and magnetic parameters for a variety of model quinones as well as the native plastoquinone cofactor of PSII (1-3). In this study, we performed density functional theory (DFT) on the reduced semiquinone state of the models in protic and aprotic solvents to determine the electronic structure, energy levels and magnetic parameters. We also created a working model of the plastoquinone pocket of PSII. The DFT calculations were optimized by using a variety of functionals and basis sets and the calculations were validated by comparison with the experimental electro-chemical properties.

1. Weyers et al., 2009, JPC B, 113, 15409.

2. Chatterjee et al., 2012, JPC B, 116, 676.

3. Chatterjee et al., 2011, Biochemistry, 50, 491.

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