Abstract Submitted
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Modeling study the mechanism of DNA repair by the photolyase proteins[1] KARL JAMES JALKANEN, Technical University of Denmark, Quantum Protein (QuP) Center — A modeling study of the mechanism of DNA repair by the photolyase proteins has been initiated. The effects of the environment on the efficiency of the repair process have been investigated. The hybrid Becke 3LYP exchange correlation functional within density functional theory has been used to model the system. The damaged species we have modeled are the cyclobutane thymine dimer, the oxetane thymine dimer and the 6,4-photoproduct (connected by only a single bond). The effects of reduction of the three damaged species and the undamaged DNA species has been investigated. For the two ring structures, reduction induces a barrierless ring opening. This supports the previously proposed model which hypothesizes that the photoreduced flavin cofactor transfers an electron (reduces) to the damaged DNA bases and with the help of the protein environment, induces the photorectivation repair process. We propose the combined use of VA, VCD, Raman and ROA spectroscopies to experimentally probe these structural changes in the DNA, the protein and the environment [1]. [1] W.-G. Han, K.J. Jalkanen, M. Elstner and S. Suhai, J. Phys. Chem. B 102 (1998) 2587.

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