MODELING ENERGY CAPTURE AND CONVERSION: CASE STUDIES OF SINGLET FISSION AND PROTON REDUCTION

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The quantum chemical modeling of two specific energy conversion processes will be discussed.

The first process involves harvesting one photon of light to yield two electrons and two holes, termed singlet fission. Singlet fission occurring in organic crystals such as pentacene and tetracene is modeled [1] using efficient new electronic structure methods for bielectronic excited states [2]. A conical intersection is shown to be responsible for the process, and details of the key bright and dark states are elucidated.

The second process is electrocatalytic proton reduction, based on a homogeneous Mo-oxo penta-pyridine catalyst recently developed in the groups of Jeff Long and Chris Chang at Berkeley [3]. Extensive computational modeling, together with new experimental measurements are employed to understand the mechanism of catalysis, and to assess the ability to tune its performance using ligand substitutions [4].

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(3) Karunadasa, H. I.; Chang, C. J.; Long, J. R. *Nature* **2010**, *464*, 1329–33.
(4) Sundstrom, E.J; Yang, X.; Thoi, V.S.; Karunadasa, H.I.; Chang, C.J.; Long, J.R.; Head-Gordon M. (submitted for publication).