Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Models of the photosynthetic oxygen-evolving centerand electronic structure of Mn clusters GABRIEL DROBNY, MICHAL BAJDICH, LUBOS MITAS, Center for High Performance Simulation and Department of Physics, North Carolina State University — It is known that the oxidation of water to O_2 in green plants is associated with a tetramanganese complex of the photosystem II (PSII) protein-cofactor complex but the exact structure of the oxygen-evolving center (OEC) remains unknown. The recent X-ray spectroscopic studies suggest that the OEC contains a cubane-like Mn_3CaO_4 center linked to a forth Mn by an oxo-bridge. Using ab-initio methods we carry out geometry optimizations for a few models of the OEC and study their electronic properties. We consider the cubane-like Mn_3CaO_4 center, a funnel-like Mn4 core with Ca ligand and a synthetic Mn_4O_6 core structure. Possibilities for binding sites and eventual reaction paths of the water splitting are explored. Manganese clusters are recognized also as single-molecule magnets. Therefore we investigate spin properties of ground and excited states of these clusters. High spin ground states of Mn_2O_2 and Mn_4 compared to a low spin ground state of Mn_4O_4 illustrate a competition between ferromagnetic and antiferromagnetic ordering.

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Date submitted: 14 Dec 2004 Electronic form version 1.4