

Abstract Submitted
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Computational Research Needs for Renewable and Alternative Energy: Studies of Natural and Artificial Photosynthesis VICTOR BATISTA, Yale University — The atmospheric oxygen that sustains life on earth has been generated by plants during the light period of photosynthesis. At the molecular level, the reaction involves catalytic water splitting into dioxygen, protons and electrons in the subunit D1 of photosystem II (a transmembrane complex of about 20 proteins found in the thylakoid membranes of green plant chloroplasts). Both the reaction mechanism and the structure of the catalytic center responsible for this important reaction remain poorly understood. This talk will present recent advances in experimental and computational studies towards the development of rigorous models of the oxomanganese catalytic complex and the catalytic cycle responsible for oxygen evolution, as well as recent progress on studies of biomimetic systems for artificial photosynthesis.

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