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Physical Chemistry of TiO₂ functionalized with oxo-manganese catalysts SABAS G. ABUABARA, CLYDE W. CADY, JIM M. SCHLEICHER, JASON BAXTER, GARY W. BRUDVIG, ROBERT H. CRABTREE, CHARLES A. SCHMUTTENMAER, VICTOR S. BATISTA, Department of Chemistry, Yale University, P.O.Box 208107, New Haven, Connecticut 06520-8107, U.S.A. — We describe the development and application of dye-sensitized semiconductors to heterogeneous photocatalysis. *Ab initio*-DFT electronic structure calculations and molecular dynamics simulations combined with quantum dynamics propagation of transient electronic excitations indicate that a surface complex consisting of a catalytic Mn oxo complex adsorbed onto a TiO₂ substrate via a catechol-substituted terpyridine ligand can be activated by photoinduced subpicosecond interfacial electron transfer. Experimental realization of the Mn oxo surface complex, achieved by a novel sequential synthesis technique, is briefly described and computational results supporting the spectroscopic characterization of the nanoscale assembly are presented. Studying the photocatalytic reaction dynamics of these uniquely functionalized semiconductor materials offers the prospect of gaining unprecedented control over a wide range of contrathermodynamic reactions. Furthermore, such biomimetic materials capable of splitting water or fixating CO₂ could provide viable solutions to problems ranging from current energy concerns to reducing atmospheric greenhouse gases.

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