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Finding hot atoms on a cold substrate: a Manganese Oxide Cluster Decorated with Water JIANWEI SUN, Univ of Texas, El Paso, MARK PEDERSON, Johns Hopkins University — Direct conversion of solar energy to fuel is the most beneficial for energy storage and distribution. In naturally occurring photosynthetic systems, it is often the case that an evolutionary designed system has both chromophores, responsible for absorbing light, and a separate reaction center where the absorbed energy is quickly transferred for conversion into chemical energy. It is not immediately clear whether nature has made such choices to avoid radiation damage near the reaction center or due to constraints that biologically assembled energy conversion systems cannot use the Aldrich catalog of chemicals. Thus, a reasonable paradigm is to search over all possible chemical systems and only consider photocatalysts for which the reaction center coincides with the chromophore or is the immediate effective recipient of sunlight through fast first-order stimulated desorptions. Here we propose a general scheme to high-throughput search for stable "cold" substrates which have "hot" reaction centers that localize the photo-induced electronic state and are in close proximity to a pair of reactants, capable of producing a desired product (possibly H_2, O_2, NH_3, or a hydrocarbon). We use a manganese oxide cluster decorated with water as an example to illustrate the scheme.

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