

Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Towards a Dithiocarbamate Ligand for CdS Nanoparticle-based Photocatalysis ANDREW O'HARA, Department of Physics and Astronomy, Vanderbilt University, ANDREW D. LACROIX, Department of Chemistry, Vanderbilt University, SOKRATES T. PANTELIDES, Department of Physics and Astronomy, Vanderbilt University, JANET E. MACDONALD, Department of Chemistry, Vanderbilt University — Photocatalysis of water into H₂ and O₂ presents a clean, renewable route for energy storage and production. Traditionally, most semiconducting nanoparticle research on photocatalysis has focused on the ability to reduce chemical systems using the photoexcited electron. Here we employ a combination of theory and experiments to develop a possible route towards the oxidation of chemical systems via the hole from photoexcitation using an asymmetric bipyridine ligand with conjugated dithiocarbamate ligand bound to the surface of cadmium sulfide nanorods. In particular, we use density functional theory to calculate the electronic levels and optical absorption of the designer ligand, free from the cadmium sulfide surface as well as attached to the surface, with and without the copper center. These calculations are compared with experimental UV/VIS absorption and fluorescence spectroscopy measurements to understand the role of copper chelation. Furthermore, theoretical comparisons are made with a related ligand known to oxidize water under an applied potential bias. Finally, we discuss whether we expect photocatalysis from the ligand and possible improvements to its design.

Andrew O'Hara
Department of Physics and Astronomy, Vanderbilt University

Date submitted: 05 Nov 2015

Electronic form version 1.4