Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Hybrid Density Functional Studies of a Promising Photovoltaic Material: Zinc Phosphide STEVEN DEMERS, AXEL VAN DE WALLE, Dept. of Applied Physics and Materials Science, California Institute of Technology — Although Zinc phosphide is a semiconductor which has high absorption in the visible spectrum that is made from abundant elements, its use as a low-cost photovoltaic is limited by difficulties in n-doping the material. We study this compound via Density Functional Theory calculations based upon recently developed hybrid functionals designed to accurately describes band gaps. We explore the effects of various point defects with energy levels near the fermi energy on the electronic band structure in an effort to identify suitable dopants in this system. The thermodynamic stability of these defects is also assessed.

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Date submitted: 27 Nov 2010 Electronic form version 1.4