Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

**Effect of hydrogen passivation on the electronic structure of ionic semiconductor nanostructures** HUIXIONG DENG, National Renewable Energy Laboratory, SHU-SHEN LI, JINGBO LI, Institute of Semiconductors, Chinese Academy of Sciences, SU-HUAI WEI, National Renewable Energy Laboratory, INSTITUTE OF SEMICONDUCTORS, CHINESE ACADEMY OF SCIENCES COLLABORATION — In theoretical studies of thin film and nanostructured semiconductors, pseudohydrogen (PH) is widely used to passivate the surface dangling bonds. Based on these calculations, it is often believed that nanostructured semiconductors, due to quantum confinement, have a larger band gap than their bulk counterparts. Using first- principles band structure theory calculation and comparing systematically the differences between PH-passivated and real-hydrogen–passivated (RH-passivated) semiconductor surfaces and nanocrystals, we show that, unlike PH passivation that always increases the band gap with respect to the bulk value, RH passivation of the nanostructured semiconductors can either increase or decrease the band gap, depending on the ionicity of the nanocompounds. The difference between PH and RH passivations decreases when the covalency of the semiconductor increases and can be explained using a band coupling model. This observation greatly increases the tunability of nanostructured semiconductor properties, especially for wide-gap ionic semiconductors.

Huixiong Deng
National Renewable Energy Laboratory

Date submitted: 14 Nov 2012 Electronic form version 1.4