Abstract Submitted
for the MAR15 Meeting of
The American Physical Society

Discrete energy bands in bulk semiconductors MAOHUA DU, HONGLIANG SHI, Oak Ridge National Lab — Bulk semiconductors typically have continuous valence and conduction bands. Discrete energy levels and bands have been sought after for various applications. For instance, discrete energy levels existing in semiconductor nanocrystals, or quantum does (QDs) have been proposed as a mechanism to suppress hot carrier thermalization and to enhance carrier multiplication in QD solar cells. Impurity bands in the band gap have been introduced for intermediate-band solar cells and for efficient visible light absorption and photocatalysis. In this talk, we show by first principles calculations that, in a multinary compound, a combination of large electronegativity difference between different cations (anions) and large nearest-neighbor distances in cation (anion) sublattices can lead to the splitting of the conduction (valence) band, resulting in several discrete and narrow energy bands separated by large energy gaps. We also discuss applications that may benefit from such electronic structure.

Maohua Du
Oak Ridge National Lab

Date submitted: 14 Nov 2014 Electronic form version 1.4