Theoretical/computational studies discover a novel three-atom-thick single-layer sheet of ZnSe that is stabilized by its unusual square lattice configuration and offers improved optoelectronic properties. Novel two-dimensional (2D) colloidal nanocrystals of semiconducting binary cadmium or zinc chalcogenides CdX and ZnX (X = S, Se, or Te) in different thicknesses are of considerable interest due to their intrinsic property tunability and potential suitability for a broad range of applications. These 2D nanocrystals demonstrate a dimensional reduction distinct from other low-dimensional materials such as 0D quantum dots and 1D quantum wires, and typically display thickness-dependent absorption and emission spectra. Indeed, the computationally discovered ultrathin sheet of ZnSe displays a quantum confinement effect stronger than the other forms of ZnSe and should have superior incident photon-to-current conversion efficiency for solar water splitting, among a wealth of potential applications. We also hypothesize that the results presented for ZnSe may be generalized to other group II-VI analogues thereby guiding discovery of new classes of semiconductor photoelectrode materials.

Reference
“A Novel and Functional Single-Layer Sheet of ZnSe”
Jia Zhou, Bobby G. Sumpter, Paul R. C. Kent, Jingsong Huang
ACS Applied Materials & Interfaces 2015, DOI: 10.1021/am505655m

Acknowledgment of Support
This research was conducted at the Center for Nanophase Materials Sciences, which is sponsored at Oak Ridge National Laboratory by the Division of Scientific User Facilities, U.S. Department of Energy.