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Tuning the electronic structure of II-VI semiconductors and nanostructures for energy applications

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Using first-principles calculations within density functional theory (DFT), we study the impacts of quantum confinement, strain, and surface ligand passivation on the electronic structure of typical II-VI wurtzite semiconductors and nanostructures. In CdSe/CdTe core/shell nanowires, large anisotropic strains develop due to the large lattice mismatch. These strains result in significant reductions in band gap in the CdSe core with increasing CdTe shell thickness, by amounts comparable to that expected from reduced quantum confinement [1]. The response of band gaps of wurtzite compounds to anisotropic strain is further shown to be large and highly non-linear, and system-dependent [2]. In addition, we also explore the effects of chemisorbed ligand on the electronic structure of CdSe surfaces. Substantial shifts in band edge energies are predicted due to the induced dipole at the CdSe-ligand interface and the intrinsic dipole of the ligand [3]. Our studies suggest well-defined routes to control both the band gaps and band edge energies of nanomaterials for light-harvesting applications.

[1] S. Yang, D. Prendergast, and J. B. Neaton, *Nano Lett.* 10, 3156 (2010).

[2] S. Yang, D. Prendergast, and J. B. Neaton, *Appl. Phys. Lett.*, in press (2011).

[3] S. Yang, D. Prendergast, and J. B. Neaton, in preparation (2011).