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Tuning Semiconductor Band Edge Energies via Surface Ligand Passivation[1] SHENYUAN YANG, DAVID PRENDERGAST, JEFFREY NEATON, Molecular Foundry, Lawrence Berkeley National Laboratory — Semiconductor band gaps and band edge energies are key parameters that can dictate the efficiency of photocatalysis in solar energy conversion applications. CdSe is a representative semiconducting system with an ideal band gap for solar photon absorption, but with band edge energies that are not positioned for efficient water splitting. Using first-principles calculations within density functional theory, we present a study of the electronic structure of passivated CdSe surfaces and nanostructures, exploring the ability to tune band edge energies in this system via chemisorbed ligands. We predict substantial shifts in band edge energies that are electrostatic in origin, and due to the induced dipole at the CdSe-ligand interface and the intrinsic dipole of the ligand. We further show that, by changing the size and orientation of the ligand's intrinsic dipole moment via novel functionalization strategies, we can control the magnitude and direction of the shifts of CdSe energy levels. The effect of ligands on energy levels of two-dimensional CdSe surfaces and nanocrystal surfaces are thoroughly discussed.

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