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Electronic Level Alignment in Multicomponent CdSe/CdTe Nanostructures from First Principles[1] SHENYUAN YANG, DAVID PRENDERGAST, JEFFREY NEATON, Molecular Foundry, Lawrence Berkeley National Laboratory — Inorganic CdSe/CdTe nanorod heterojunctions, with type-II level alignment and band gaps in the solar spectrum, comprise ideal model components of nanostructure-based solar cells. Here we perform density functional theory calculations on CdSe/CdTe nanowire heterojunctions, exploring how the electronic properties of their nanoscale interfaces are affected by quantum confinement, and mechanical and electrical boundary conditions. Many-body perturbation theory within the GW approximation is used to predict quantitative bulk band gaps and infer bulk level alignment. We find that band offsets at bulk epitaxial interfaces are quite sensitive to biaxial strain due to lattice mismatch. The computed band gaps of small linear nanorod heterojunctions increase with decreasing diameter due to quantum confinement, but band offsets are seen to be largely unaffected. In the core/shell nanorod heterojunctions, band offsets are strongly dependent on strain and confinement, both of which can be tuned by the core size and shell thickness.

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