

**COMPARATIVE STUDY OF THE STRUCTURE AND ELECTRONIC PROPERTIES
OF BILAYER CdSe-CdS AND CdTe-CdS QUANTUM DOTS AND QUANTUM WELLS
BY AB INITIO CLUSTER AND FIRST-PRINCIPLES SLAB CALCULATIONS**

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Semiconductor nanoparticles and nanofilms find increasing use as efficient converters of electric energy to light (light-emitting devices) and light to electric energy (solar cells), as quantum dots in self-assembled quantum-dot arrays, as quantum wells in heterojunctions, and in many other electronic, photonic, and spintronic applications. In this work, CdS, CdSe and CdTe single-component nanostructures and CdSe-CdS and CdTe-CdS bilayer (core/shell) systems with the wider bandgap semiconductor as the shell and the narrower bandgap semiconductor as the core are studied theoretically using ab initio cluster and first-principles slab calculations. The structure and most important electronic properties (work function, band structure, etc.) are calculated and analyzed. The spectral properties of these nanostructures are analyzed.