Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

SUPPORTING INFORMATION

Bulk and surface properties investigation of CdSe: insights from theory

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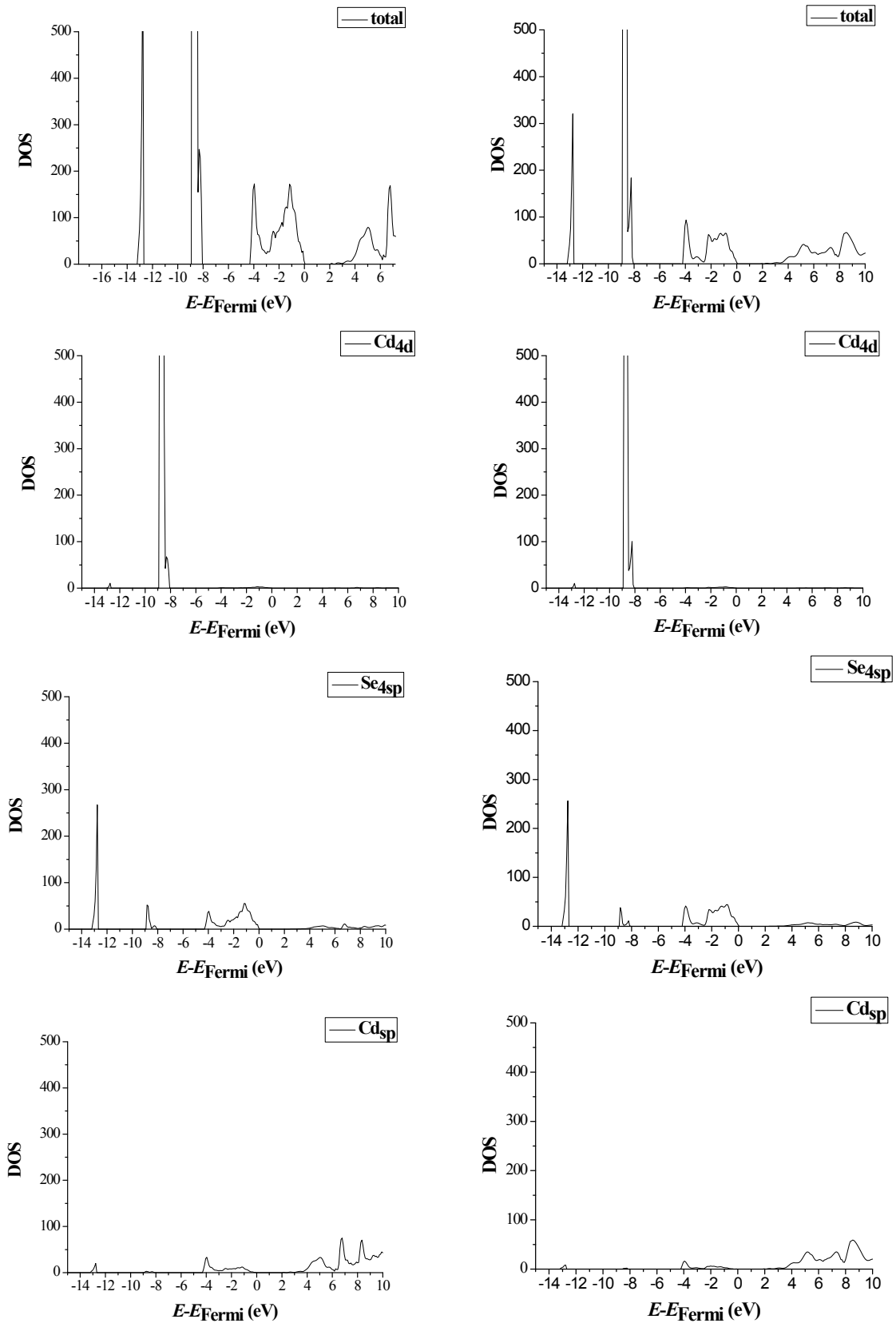

Figure S1. Calculated total and orbital-projected density of states of the CdSe wurtzite (left) and zinc blende (right) bulk crystals. Fermi level was set at 0 eV.

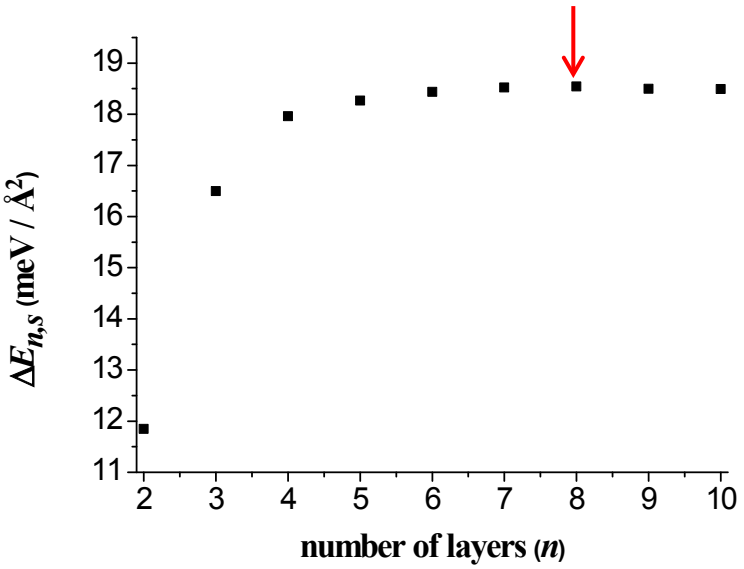

Figure S2. Calculated surface formation energies for the (10-10) surface as a function of the number of layers of CdSe wurtzite slabs. Convergence (indicated by a red arrow) is reached at 8 layers.

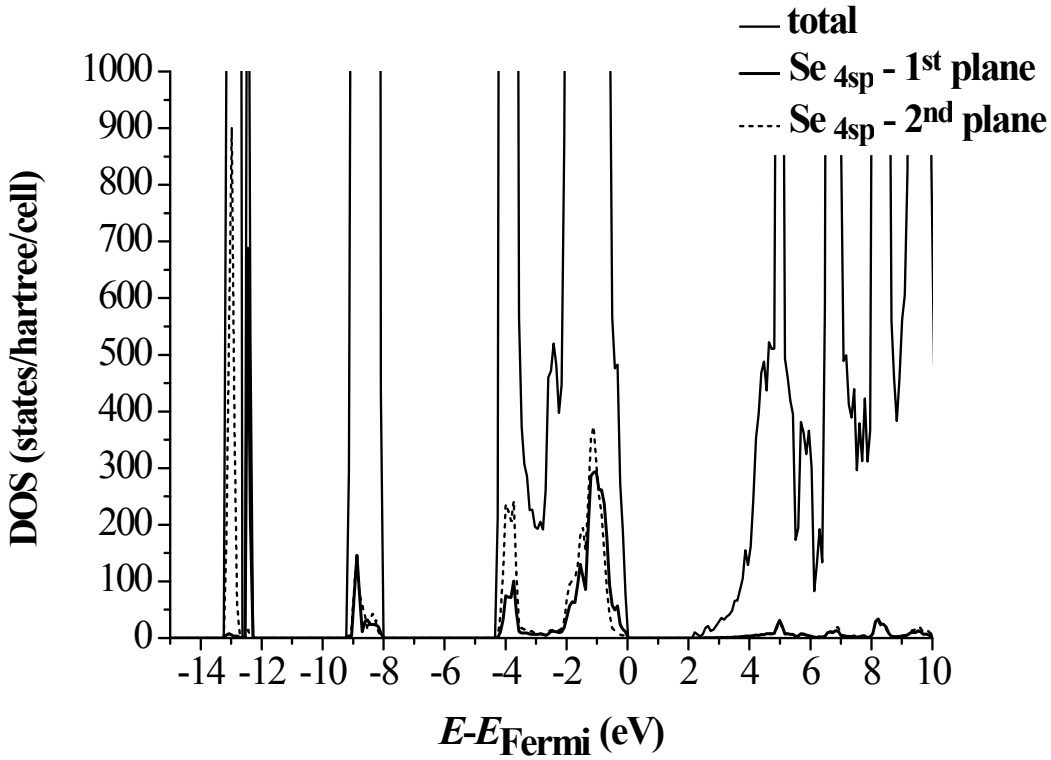

Figure S3. Computed total and orbital-projected density of states of the CdSe wurtzite (10-10) surface obtained for an 8 layer thick slab. Fermi level was set at 0 eV.