Supporting Information

A New Ab-Initio-Based Pair Potential for Accurate Simulation of Phase Transitions in ZnO

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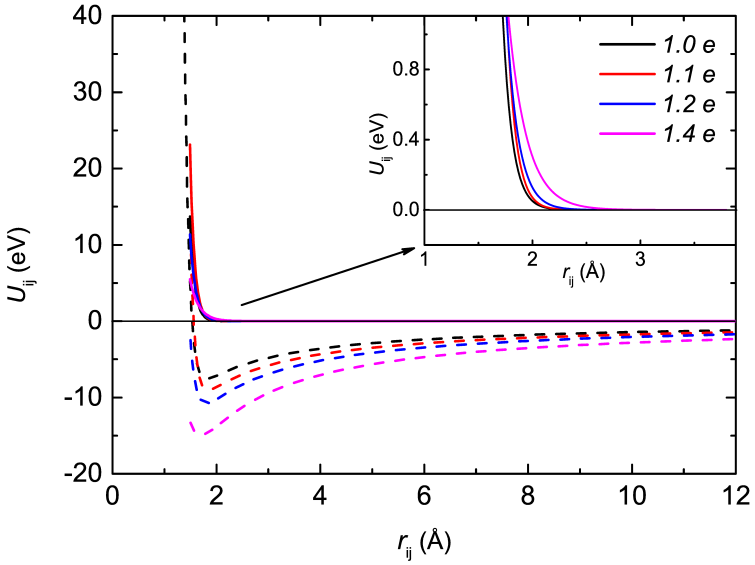

Figure S1: Short-range (solid lines) and total (dashed lines) interaction potentials of the Zn-O interaction with effective charges of 1.0, 1.1, 1.2, and 1.4 e. The upper-right inset shows a magnification of the short-range interaction potentials.

Computational details of the DFT calculations for some II-VI semiconductors

First principles density functional theory calculations for ZnS, CdS, and CdSe were performed using the VASP code.[1] Within the projected augmented wave (PAW) method[2] the generalized gradient approximation (GGA) functionals by Perdew, Burke and Ernzerhof[3] (PBE) were used. The cut-off energy was set to a relatively high value of 600.0 eV, while the cut-off of the augmentation waves was set to 900.0 eV. Calculations were performed for three phases: the wurtzite (WZ), rock salt (RS), and honeycomb (HC) crystal structures. For the conventional unit cell of RS, a Monkhorst Pack k-mesh of $24 \times 24 \times 24$ was used. For the hexagonal WZ and HC structures, gamma centered k-point meshes of $30 \times 30 \times 26$ and $30 \times 30 \times 30$, respectively, were used. A scan over cut off energies and k-point meshes showed that the results are well converged within 0.5 meV/atom.

Lattice parameters and the relative stabilities

Lattice parameters and the relative stabilities of ZnS, CdS, and CdSe in the WZ, RS and HC structures are listed in Table S1, together with the results for ZnO. $\Delta E_{\mathrm{HC-WZ}}$ and $\Delta E_{\mathrm{RS-WZ}}$ are the energy differences of the HC and RS structures with respect to the WZ structure, respectively. The ratio ρ, where $\rho = \Delta E_{\mathrm{HC-WZ}}/\Delta E_{\mathrm{RS-WZ}}$ under zero temperature and zero pressure conditions was also calculated and is listed for each material. Among these four II-VI semiconductors, ZnO has the smallest values of $\Delta E_{\mathrm{HC-WZ}}$ and ρ. Therefore, ZnO may be the best candidate to find stabilized HC structure in experiments.

Table S1: Lattice parameters and the relative stabilities of ZnO, ZnS, CdS, and CdSe in the WZ, RS, and HC structures computed by DFT. Lattice parameters a and c are in Å; the energy difference ΔE is in eV/f.u.; The ratio ρ is defined as $\rho = \Delta E_{\mathrm{HC-WZ}}/\Delta E_{\mathrm{RS-WZ}}$.

	ZnO	ZnS	CdS	CdSe
wurtzite, Space group $P6_3mc$ (No. 186)				
a	3.287	3.850	4.205	4.392
c	5.306	6.314	6.845	7.171
rock salt, Space group $Fm\bar{3}m$ (No. 225)				
a	4.337	5.108	5.505	5.748
ΔE_{RS-WZ}	0.294	0.626	0.268	0.290
honeycomb, Space group $P6_3/mmc$ (No. 194)				
a	3.465	3.985	4.448	4.656
c	4.580	5.976	5.822	6.069
ΔE_{HC-WZ}	0.138	0.332	0.180	0.208
ρ	0.469	0.530	0.672	0.717

References

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