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Supplementary Material for "Alloy Disorder and Partial Order Effects on the Bowing Parameter of CdZnTe Semiconductors"

by Kan Luo[1], Louis Rossignol[1], Piotr Jakuc[1], Oussama Moutanabbir[2] and Hong Guo[1]

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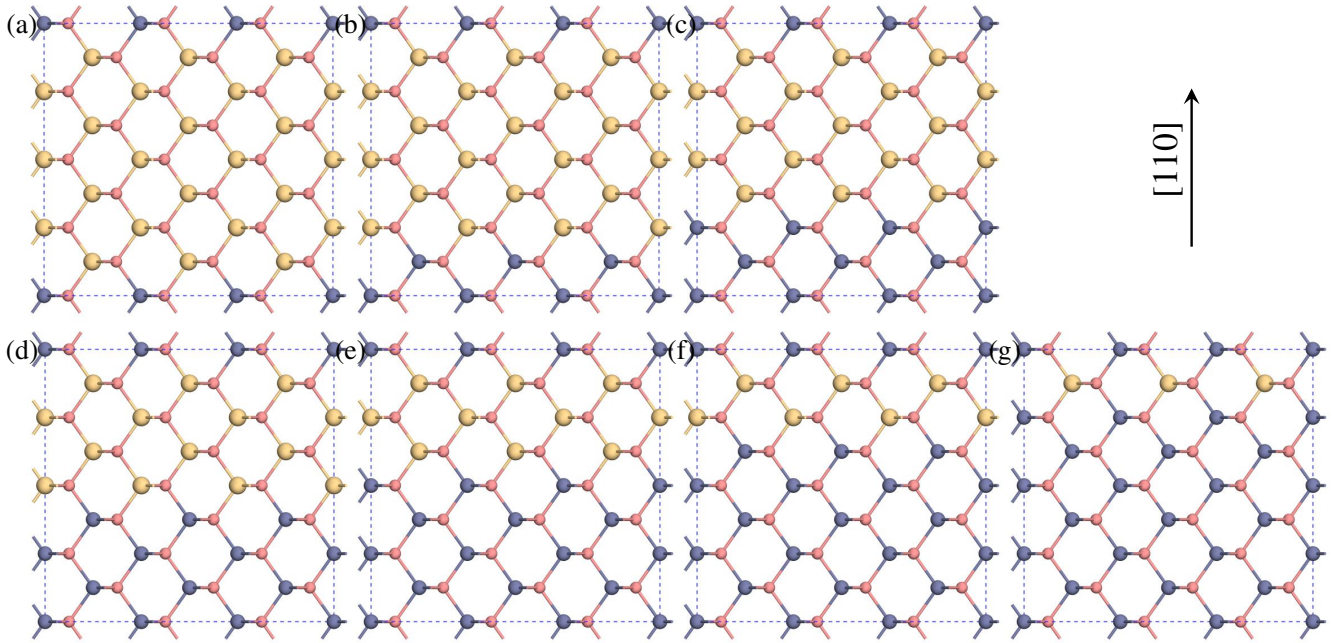


FIG. S1. The partially ordered structures along [110] direction with the Zn content x values of 1/8 (a), 1/4 (b), 3/8 (c), 1/2 (d), 5/8 (e), 2/3 (f) and 7/8 (g), respectively.

Alt text: Seven atomic-structure renderings of partially ordered CdZnTe supercells along the [110] direction for Zn fractions $x = 1/8$, 1/4, 3/8, 1/2, 5/8, 2/3, and 7/8. Increasing Zn content progressively enlarges the ZnTe-rich region and shifts the ZnTe/CdTe interface through the supercell.

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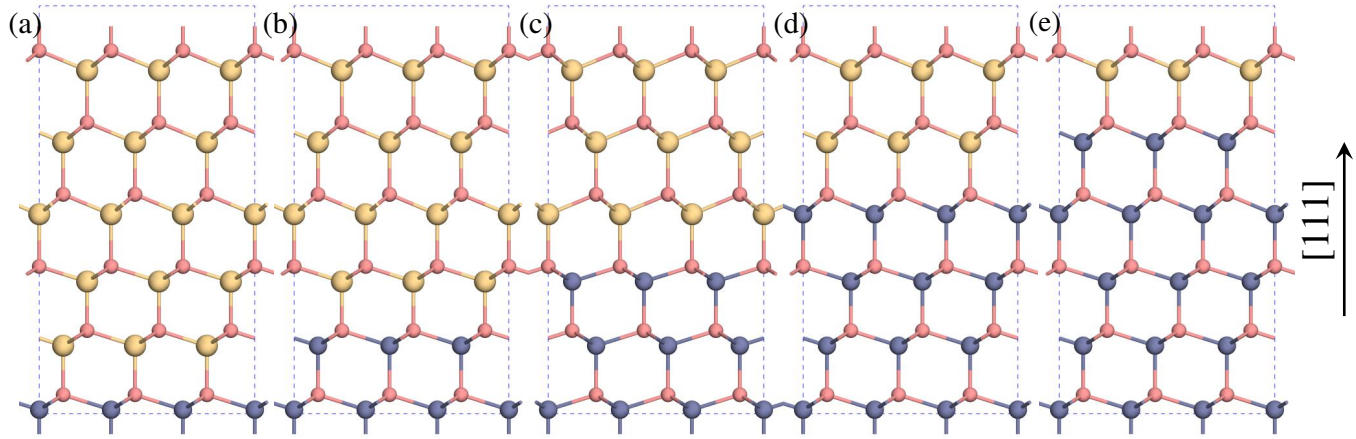


FIG. S2. The partially ordered structures along [111] direction with the Zn content x values of 1/6 (a), 1/3 (b), 1/2 (c), 2/3 (d) and 5/6 (e), respectively.

Alt text: Five atomic-structure renderings of partially ordered CdZnTe supercells along the [111] direction for Zn fractions $x = 1/6$, $1/3$, $1/2$, $2/3$, and $5/6$. The ZnTe-rich portion increases with composition, producing progressively larger compositionally segregated regions separated from CdTe across a [111]-oriented interface.

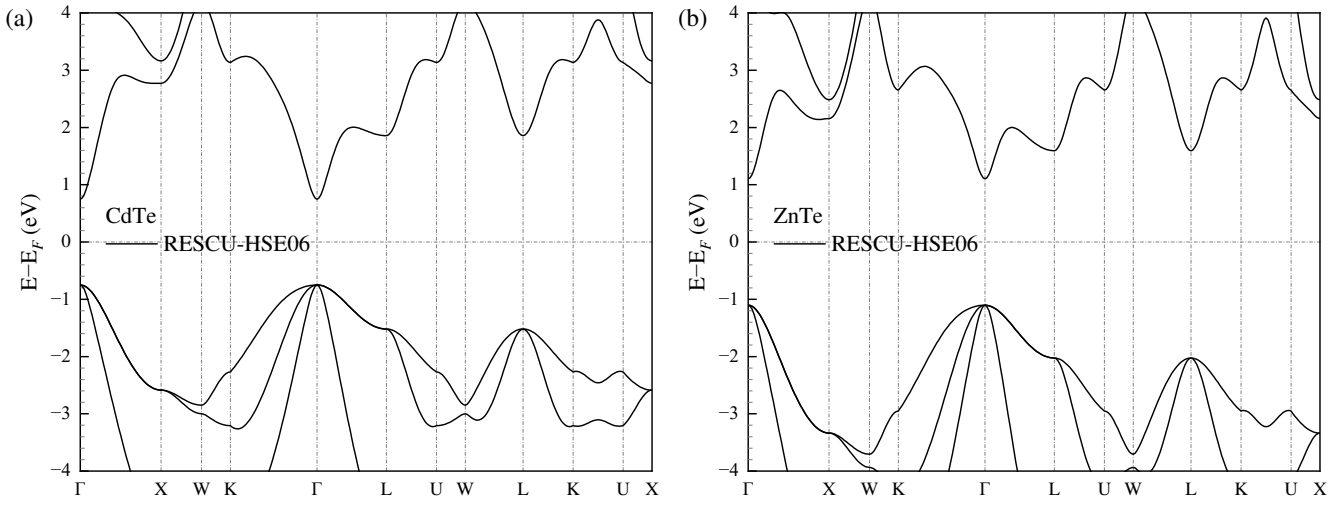


FIG. S3. The band structures of CdTe (a) and ZnTe (b) primitive cells calculated using RESCU within the HSE06 functional.

Alt text: Two electronic band-structure plots compare CdTe and ZnTe primitive cells calculated using RESCU-HSE06 along the same sequence of high-symmetry crystal directions. Both show separated valence and conduction bands around the Fermi level, with ZnTe exhibiting a larger band gap than CdTe.

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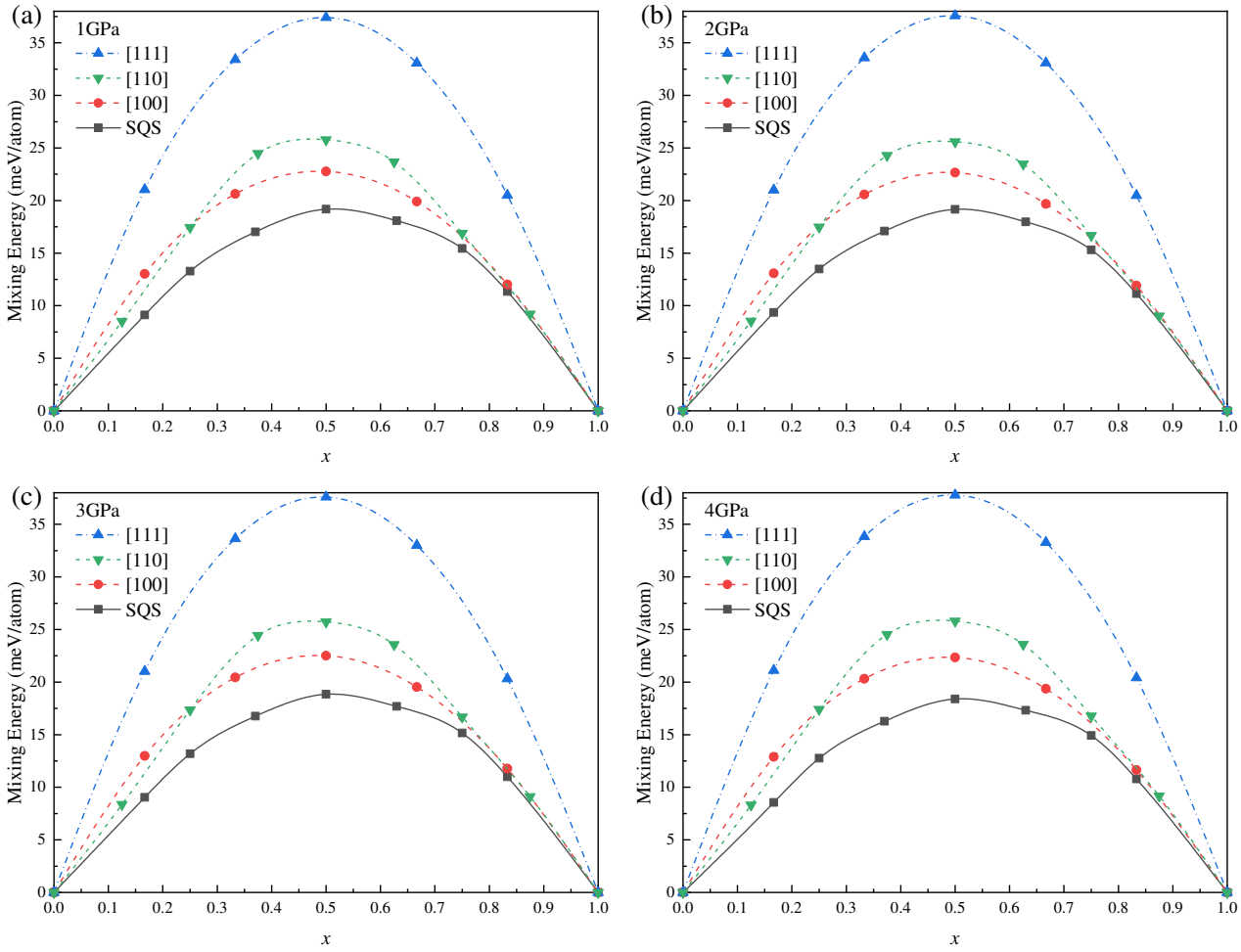


FIG. S4. The mixing energy of the disordered and partially ordered CZT with pressures under 1 GPa (a), 2 GPa (b), 3 GPa (c) and 4 GPa (d), including the interface models along [100], [110] and [111] directions, presented as a function of Zn content x.

Alt text: Four plots show CZT mixing energy versus Zn content at pressures of 1, 2, 3, and 4 GPa for SQS and partially ordered [100], [110], and [111] structures. Mixing energy peaks near intermediate composition, is lowest for SQS structures and highest for [111] interfaces, and changes little with pressure.

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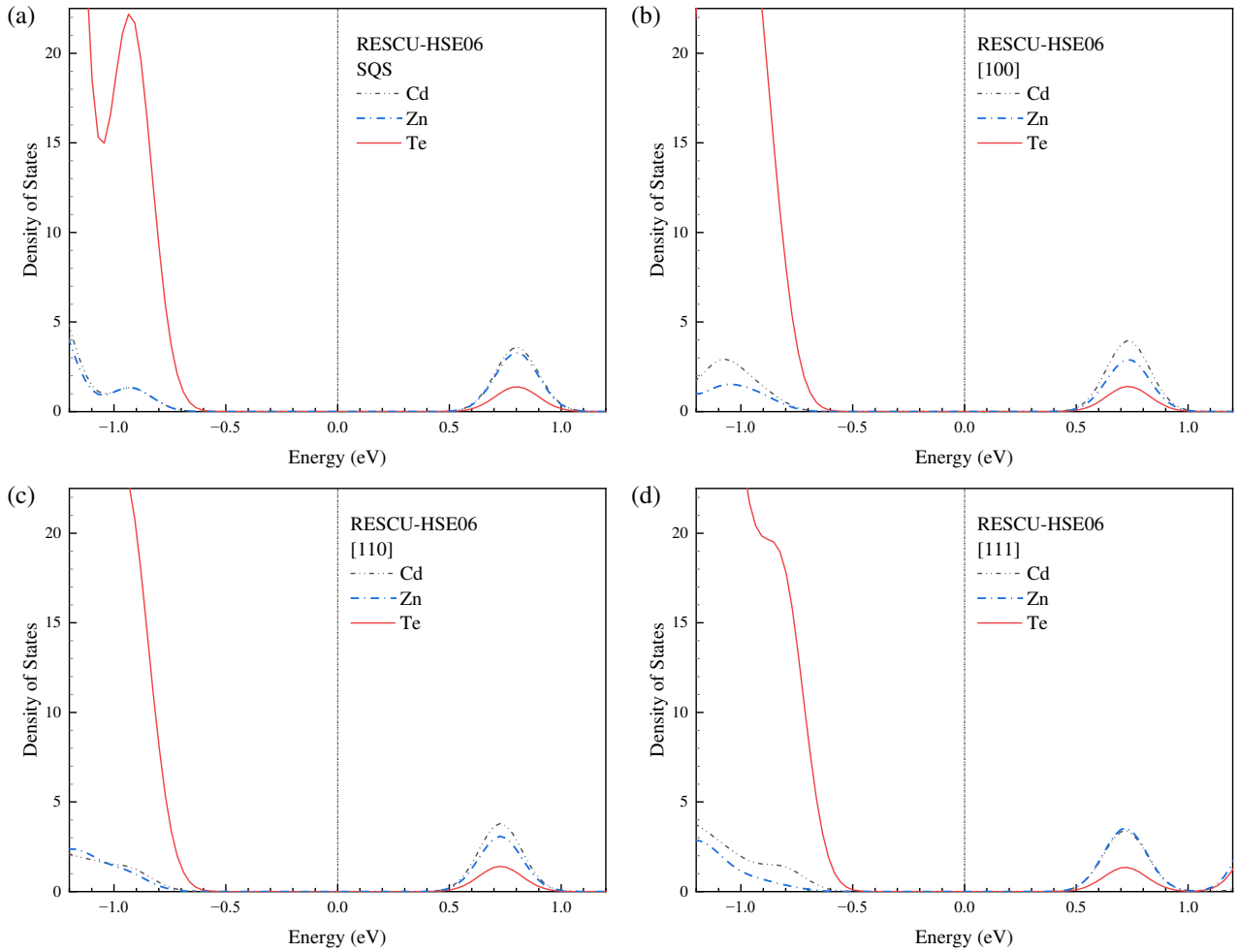


FIG. S5. The density of states for $Cd_{0.5}Zn_{0.5}Te$ SQS (a) and PO-configurations along [100] (b), [110] (c) and [111] (d) directions.

Alt text: Four density-of-states plots compare Cd, Zn, and Te contributions in $Cd_{0.5}Zn_{0.5}Te$ for the SQS structure and partially ordered [100], [110], and [111] configurations. The atomic contributions near the band edges differ between disordered and partially ordered structures, particularly the Cd contribution in the valence-band region.