Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Supplementary Information

Impact of vacancy defects and element substitution on the electrical transport properties of θ-Al_2Cu and θ_c'-Al_2Cu: A NEGF-DFT Study

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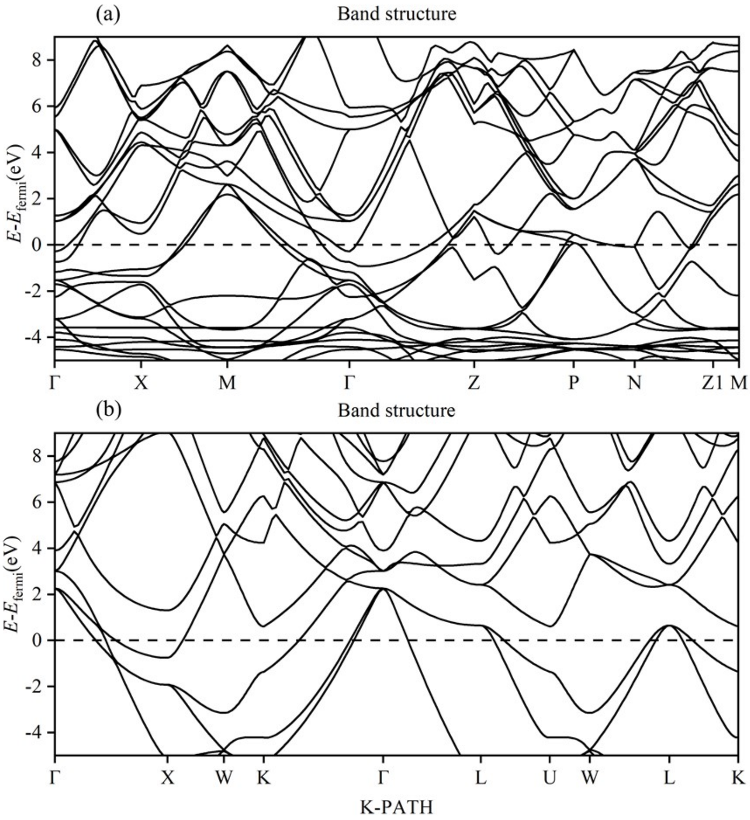

FIG. S1. Band structure diagrams of (a) bct and (b) fcc crystals.

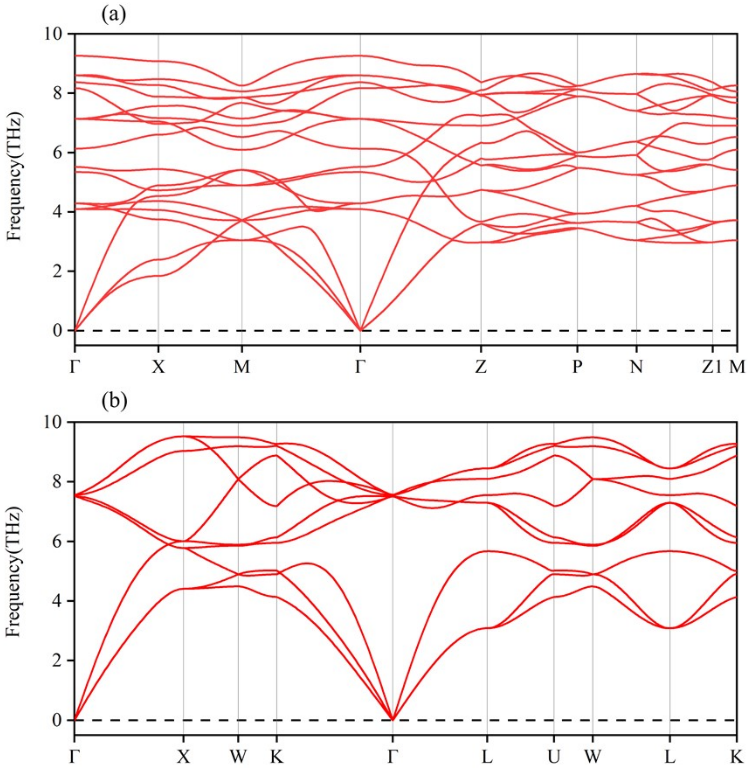

FIG. S2. Phonon spectra of (a) bct and (b) fcc crystals.

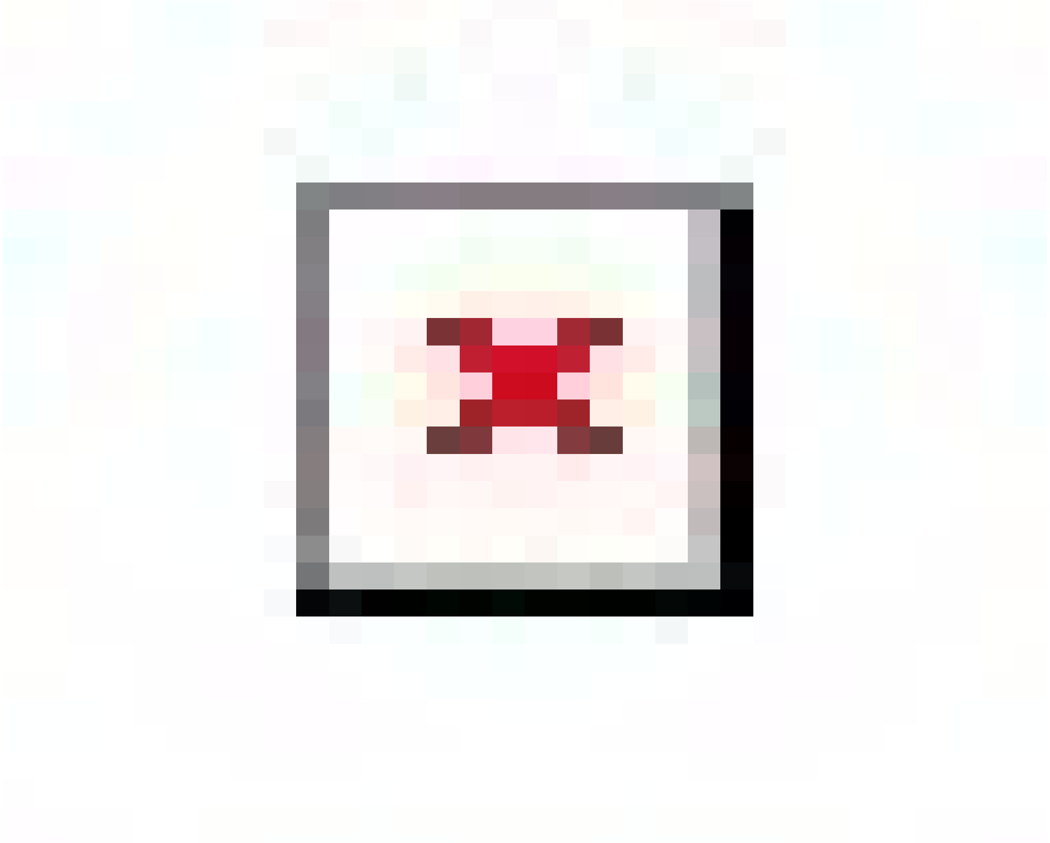

FIG. S3. The projection diagrams display the effective potential differences of the substitutional defect structures of the two systems along the real space transport direction.

FIG. S4. Plots of the distribution of the difference in the local density of states along the transport direction z for the perfect and vacancy systems. Panels (a) and (b) correspond to the bct-Systems, while panels (c) and (d) represent the fcc-Systems. The black dotted line is the Fermi level.

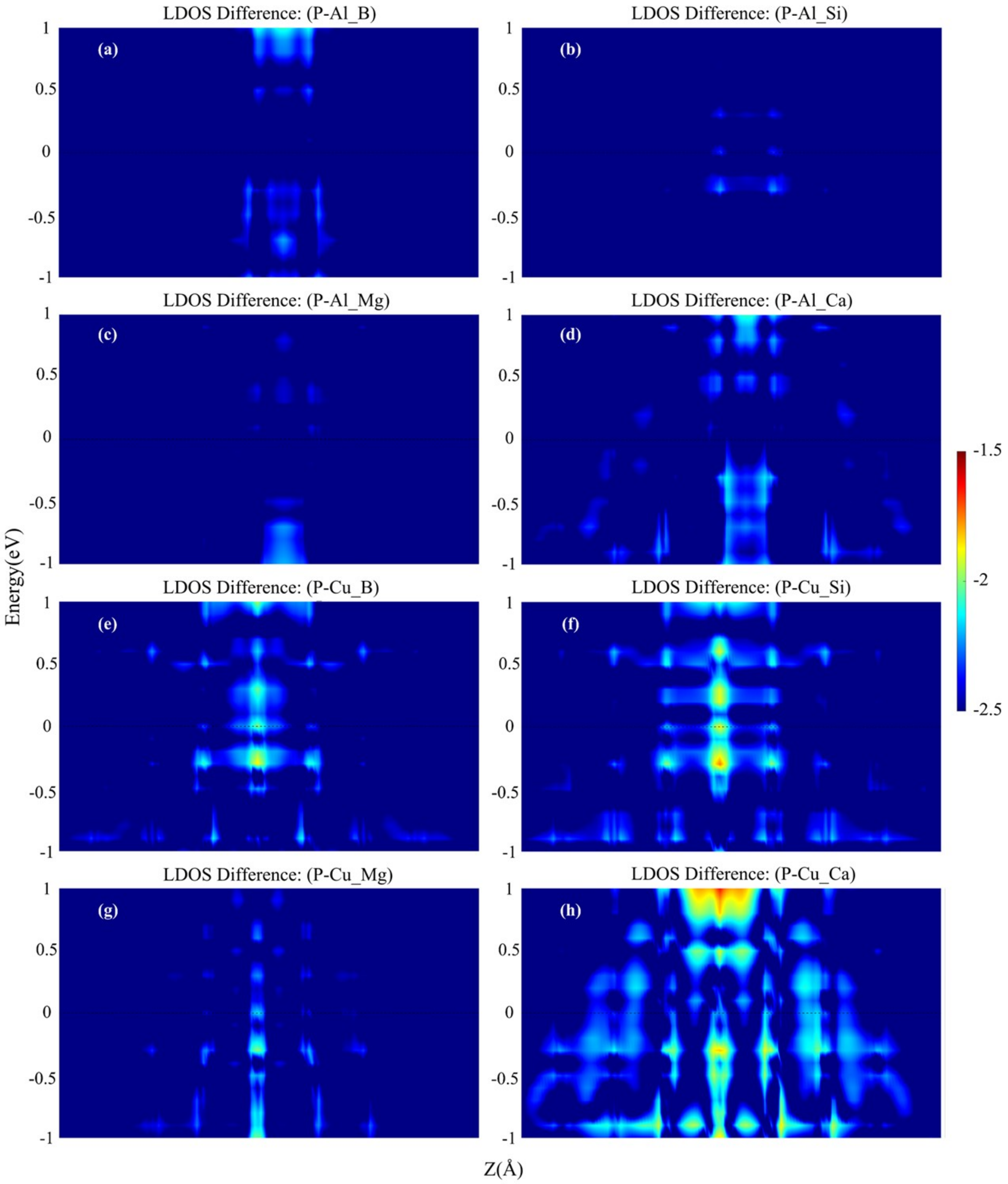

FIG. S5. The distribution of the difference in LDOS between the perfect system and the substitutional defect systems in bct-Systems along the transport direction z is shown, where (a)-(d) are the difference plots between the perfect system and the Al_X systems, and (e)-(h) are the difference plots between the perfect system and the Cu_X systems.

FIG. S6. The distribution of the difference in LDOS between the perfect system and the substitutional defect systems in fcc-Systems along the transport direction z is shown, where (a)-(d) are the difference plots between the perfect system and the Al_X systems, and (e)-(h) are the difference plots between the perfect system and the Cu_X systems.