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Pressure-induced structural phase transition of zinc oxide

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Abstract content
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The high-pressure technique is useful to understand physical properties because the technique can directly control bond length and phase transition. As a general trend, the pressure-induced phase transition causes an increase of coordination number with a drastic change of their physical properties. Here, we attempt to explore the pressure-induced phase transition from the sixfold-coordinated NaCl structure (B1) to the eightfold-coordinated CsCl structure (B2) in CdO by applying an effective interionic interaction potential, which includes the long range Coulomb, van der Waals (vdW) interaction and the short-range repulsive interaction upto second-neighbor ions within the Hafemeister and Flygare approach. Assuming that both the ions are polarizable, the Slater-Kirkwood variational method is employed to estimate the vdW coefficients for CdO. The estimated value of the phase transition pressure (Pt) and vast volume discontinuity in pressure volume phase diagram identifies the structural phase transition from B1 to B2 structure.

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