



Contribution ID: 100

Type: Poster Presentation

Pressure-induced structural phase transition of zinc oxide

Tuesday, 12 July 2016 16:30 (1 hour)

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 (P_t) and vast volume discontinuity in pressure volume phase diagram identifies the structural phase transition from B1 to B2 structure.

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Session Classification: Poster Session