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Computational and theoretical study of Cd doped ZnO phase separation

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Abstract content
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Cd and Zn are isoelectronic transition metals, and hence CdO alloying with ZnO could manifest interesting features infused CdO-ZnO structures. Importantly, Cd doping reduces the energy bandgap and results in a red-shift of absorption edge hence, one can envision varying the Cd doping concentration to tailor the electronic gaps to produce materials of interest for UV sensors, UV LEDs, UV protecting layers. Incorporation of Cd into ZnO produces a material with increased conductivity and increased carrier concentration versus the parent ZnO. In the present study, a direct correlation of structural and optical properties of Zn_{1-X}Cd_XO (0.55 ≤ X ≤ 0.85) has been developed both theoretically and computationally. Zn_{1-X}Cd_XO nanopowders synthesized via sol-gel route are used to compare the optical properties with computational calculations done using COMSOL MultiPhysics 5.2. The Zn_{1-X}Cd_XO nanopowder exhibits the coexistence of hexagonal ZnO and cubic CdO phase. The narrow energy gaps indicate that both hexagonal and cubic Zn_{1-X}Cd_XO systems have potential as material for solar energy applications. We give direct evidence for a chemical phase separation using X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FTIR).

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