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Improved optoelectronic properties in CdSexTe1-x through controlled composition and short-range order[1] BISHAL DUMRE, NATHAN SZYMANSKI, VIJAYA ADHIKARI, INDIRAS KHATRI, The University of Toledo, Toledo, OH, DANIEL GALL, Rensselaer Polytechnic Institute, Troy, NY, SANJAY KHARE, The University of Toledo, Toledo, OH — We employ first principles methods based on density functional theory and beyond to study CdSexTe1-x alloys in the zincblende and wurtzite structures. From the cluster expansion formalism, we provide phase diagram showing consolute temperature of 325 K where zincblende-to-wurtzite phase boundary is found for Se concentrations of x=0.5-0.6 owing to increasing ionic character of the Cd-anion bonds. Disordered CdSexTe1-x configurations are modeled using special quasirandom structures, for which optoelectronic properties are computed with the hybrid HSE06 functional. Downward bowing in the band gap and effective hole mass of the zincblende structure is highlighted for its potential benefits in photovoltaics through increased net photocurrent. Absorption coefficient and reflectivity are also reported, showing promising results in zincblende CdSexTe1-x as indicated by substantial optical absorption throughout all Se concentrations. Lastly, we identify the presence of short-range order in CdSexTe1-x characterized by clustering among like atoms in order to minimize strain. The degree of clustering, which may be tuned by temperature, also controls the magnitude of the band gap.

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