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ab initio studies of thermoelectric materials for energy conversion applications

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Abstract content
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Energy harvesting requires clean and highly efficient energy conversion technologies. Thermoelectricity is one such technology that achieves thermal-to-electric conversion and vice versa. This is achieved purely by solid state means and has a great potential for applications in waste heat recovery, air conditioning and spot cooling of electronic devices. Attempts have been directed towards exploration of high performance compounds which are yet to be realized. To predict the enhanced electronic structure of Cadmium Oxide (CdO), we doped it with Zn and Mn. The structural properties in terms of volumes and lattice parameters, the band structure and the density of state for both the doped and undoped CdO were determined by the modern ab initio methods based on density functional theory (DFT). We established that indeed doping improved thermoelectric properties of cadmium oxide.

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