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DFT Study of Skutterudite CoSb3 and In0.2Co4Sb12 Thermoelectric Heterostructures with 2D-WSe2

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Abstract

Recently, two–dimensional WSe2 transition–metal dichalcogenides have been used for novel electronic devices. However, its influence on the electronic and optical properties of thermoelectric Skutterudite CoSb3 and In0.2Co4Sb12 is unknown. Despite the increased potential of energy conversion obtained by doping CoSb3 with indium, further theoretical study is necessary to understand the origin of this enhancement. Heterostructures of hybrid WSe2/CoSb3 and WSe2/In0.2Co4Sb12 are investigated in this study using a density functional theory calculation. The electronic structure, energy, geometry optimisation and optical properties are analysed for the individual components in the heterostructure. The obtained results show that pure CoSb3 has a bandgap of 0.456 eV, and In0.2Co4Sb12 has a zero bandgap, while the calculated bandgap for WSe2 is found to be 1.482 eV. The heterostructures show an exceptional absorption in the infrared region where the heat energy mainly dominates. The charge transfer study indicates a built–in potential at the interface, which ensures easy separation of charge generated carriers and thus, improved the thermoelectric performance.