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The nature of the high thermoelectric properties of CuInX₂ (X = S, Se and Te):**First-principles study****Yang Gui(1), Lingyun Ye(3), Chao Jin(1), Jihua Zhang(2), and Yuanxu Wang(1, 2)***

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Abstract

CuInX₂ (X = S, Se and Te) are members of Cu-based compounds with diamond-like structures. Their bonding characteristics, electronic structure and thermoelectric properties are studied using first-principles methods and the semiclassical Boltzmann theory. Due to the Cu-3d orbits in CuInX₂, we use the mBJ+U method to obtain the accurate band gap and electronic structures. The analysis of the electronic structure for CuInX₂ indicates that the combination of heavy and light bands near the Fermi level is conducive to achieve high thermoelectric performances. However, few literatures have reported the reason of the combination. Further study on AgGaTe₂, CuGaTe₂, and CuInX₂ (X = S, Se and Te) shows that the stronger interaction between Cu-Te atoms leads to the combination of heavy and light bands in Cu-based compounds. These results provide a valuable theoretical guidance that the introduction of Cu-Te bonding in experimental synthesis is helpful to improve the thermoelectric properties.

Keywords: Cu-based compounds; Seebeck effect; thermoelectric properties;

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