A first principle study of thermoelectric properties of some chalcogenides materials

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Thermoelectric chalcogenide materials exhibit promising properties, making them suitable for energy conversion and cooling applications. Thermoelectric (TE) materials have attracted significant interest due to their potential for energy harvesting and conservation. For a material to be considered an efficient thermoelectric material, it must possess low thermal conductivity, high electrical conductivity, a high Seebeck coefficient, and a high power factor. These characteristics contribute to strong thermoelectric performance, leading to a favorable figure of merit (ZT). Although several promising bulk semiconductors have been reported by researchers, no satisfactorily high ZT values have yet been achieved. Chalcogenide semiconductors may provide a solution to this challenge. Using density functional theory (DFT) and Boltzmann transport theory, the thermoelectric properties of selected chalcogenide materials (Cu_2S, Cu_2Se, InS, and InSe) were analyzed. These studies revealed strong thermoelectric performance, as the predicted maximum ZT values indicated high efficiency in these materials.