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Role of Interlayer Coupling for the Power Factor of CuSbS2 and CuSbSe2

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Abstract : The electronic and transport properties of bulk and monolayer CuSbS2 and CuSbSe2 are determined by using density functional theory and semiclassical Boltzmann transport theory, in order to investigate the role of interlayer coupling for the thermoelectric properties. The calculated band gaps of the bulk compounds are in agreement with experiments and significantly higher than those of the monolayers, which thus show lower Seebeck coefficients. Since also the electrical conductivity is lower, the monolayers are characterized by lower power factors. Therefore, interlayer coupling is found to be essential for the excellent thermoelectric response of CuSbS2 and CuSbSe2, even though it is weak.

Keywords : density functional theory, thermoelectric, electronic properties, monolayer
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