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Role of the interlayer coupling for the thermoelectric properties of CuSbS2 and CuSbSe2[1] NAJEBAH ALSALEH, NIRPENDRA SINGH, UDO SCHWINGENSCHLOGL, King Abdullah University Of Science and Technology (KAUST) — The electronic and transport properties of bulk and monolayer $CuSbS_2$ and $CuSbSe_2$ are determined using density functional theory and semiclassical Boltzmann transport theory, in order to investigate the role of the 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 characterised by lower power factors. Therefore, the interlayer coupling is found to be essential for the excellent thermoelectric response of $CuSbS_2$ and $CuSbSe_2$ even though it is of weak van der Waals type.

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