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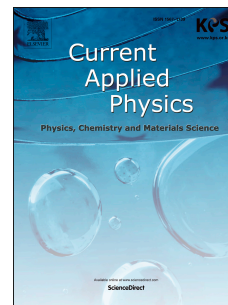
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Prediction on the physical properties of CuInS₂ with various anion positions

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Abstract: The effects of various anion displacements (u) on electronic structures, elastic constants, Debye temperature and the minimum thermal conductivity of CuInS₂ are studied by first-principles calculation. The lattice constant couples with the anion displacement, however, they are not consistent with the relation proposed by Abrahams and Bernstein. When the anion displacement varies from 0.2 to 0.3, the Cu-S bond length is elongated, while the In-S bond length is shortened, which cause the increase of band gap with anion displacement. The anisotropies of sound velocities and lattice thermal conductivities are also discussed. The results imply that the lattice thermal conductivity along [110] direction is the smallest and decreases with u . These research findings shed light on improving the thermoelectric properties by manipulating u and the direction of propagation.

Keywords: CuInS₂, electronic structures, elastic properties, first principles

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