

Phase transitions in AuTe₂ from first-principles calculations

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Abstract

We report results of first-principles calculations of calaverite, AuTe₂, a mineral that presents an incommensurate phase at low temperature and pressure.

The average structure is metallic, three electronic bands crossing the Fermi level. The average monoclinic structure presents a nesting of the Fermi surface, characterized by a \mathbf{q}_F vector $\langle -0.4076$ -0.4076 $0.4479 \rangle$, that is close to the experimentally determined \mathbf{q} vector of the incommensurate modulation.

Relaxation calculations show a pressure shift of the order of 5 GPa. The high-pressure phase is not modulated. We perform a study under pressure within a large pressure range: -5 to 75 GPa.

We observe two phase transitions. The first one appearing at about -3 GPa theoretical pressure corresponding to the trigonal (high-pressure) - to - monoclinic (low-pressure, average structure) transition, observed also experimentally. Preliminary results show an instability in the phonon dispersion spectra of the low-pressure monoclinic average structure, with an instability close to the experimentally determined \mathbf{q} vector of the incommensurate modulation.

The second phase transition is predicted at about 55 GPa to be isosymmetrical. The high-P phase (higher than 55 GPa) does not present any instability in the phonon dispersion spectra.