

Abstract Submitted
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Identification and properties of the non-cubic phase of Mg₂Pb.

YUWEI LI, GUANG BIAN, DAVID SINGH, Univ of Missouri - Columbia — Mg₂Pb is a superconducting semimetal that occurs in a cubic $Fm-3m$ structure. However, Eldridge and co-workers reported a lower symmetry structure with slight off stoichiometry, but were not able to refine. Here we identify this phase and report its properties, based on first principles calculations and structure predicting methods. We find a metallic tetragonal ($P4/nmm$) compound with interesting anisotropy. First principles total energy calculations indicate the enthalpy of $P4/nmm$ structure is only 2 meV/atom higher than that of $Fm-3m$ structure.

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