

Pressure-induced band anticrossing in two adamantine ordered-vacancy compounds: CdGa₂S₄ and HgGa₂S₄

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Abstract

This paper reports a joint experimental and theoretical study of the electronic band structure of two ordered-vacancy compounds with defect-chalcopyrite structure: CdGa₂S₄ and HgGa₂S₄. High-pressure optical-absorption experiments (up to around 17 GPa) combined with first-principles electronic band-structure calculations provide compelling evidence of strong nonlinear pressure dependence of the bandgap in both compounds. The nonlinear pressure dependence is well accounted for by the band anticrossing model that was previously established mostly for selenides with defect chalcopyrite structure. Therefore, our results on two sulfides with defect chalcopyrite structure under compression provide definitive evidence that the nonlinear pressure dependence of the direct bandgap is a common feature of adamantine ordered-vacancy compounds and does not depend on the type of anion.

Keywords: vacancy compounds, chalcopyrite structure, bandgap, band anticrossing, optical absorption experiments

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