

Anomalous pressure modulation of the lowest B_{1g} lattice vibration in semimetal zirconium diphosphide, ZrP_2

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Abstract

Lattice dynamics of ZrP_2 , a semimetal compound with non-trivial topology of electronic bands, has been studied through measurements of inelastic light scattering and extensive ab initio calculations at range of static pressures up to 20 GPa. We found that lattice vibrations of the lowest energy exhibited anomalous properties.

An abnormal change in the energy of the lowest B_{1g} phonon mode revealing alternate softening (energy decrease) and hardening (energy increase) regimes has been observed within 16 GPa pressure range. This finding substantially complements the very recent observation of the softening of the lowest A_g lattice mode in $ZrPAs_2$ [1] and ZrP_2 [2] under compression. Our study demonstrates a complex behavior of optically active lattice vibrations, the reason for which is yet to be understood.

In a broader context, detecting lattice instability manifested through the soft phonon modes in the low energy region might be of high relevance to the mechanism of driving superconductive state observed recently in several semimetal compounds under compression urging for further scrupulous investigation.

References:

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