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First-Principles Study of the Physical Properties of CuV_2S_4 under Pressure

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The structural, electronic, mechanical, thermodynamic, and optical properties of CuV_2S_4 have been studied under pressure $(0-50\,\text{GPa})$ by employing first-principles computation depending on the density functional theory. The optimized structural constraints are in good accord with the experimental results. By employing different pressure, the variation of single crystal elastic constant C_{ij} as well as polycrystalline mechanical parameters are evaluated and discussed in detail. The increment of elastic constant with the increase in pressure guaranteed that CuV_2S_4 turn ought to be more resilient to shear distortion with pressure. The linear response of elastic moduli under pressure confirms that CuV_2S_4 hardness rises with increasing pressure. The Pugh's ratio ensured the ductile nature of CuV_2S_4. Band structure and DoS calculations have been confirmed the electrically conductive nature of CuV_2S_4. The population analysis validates the presence of dominant covalent bonding. Optical properties, *i.e.*, absorption, conductivity, reflectivity, and loss function are also explored with the variation of pressure. These optical functions demonstrate that the compound exhibits high reflectivity in the low-energy range, which assures the application of this compound as coating material. The thermodynamic properties are also investigated under pressure and discussed.

Keywords: first-principles study, spinel-type compound CuV_2S_4, mechanical properties, electronic properties, optical and thermal properties.