Lattice dynamics and optical properties of GeS from first principles

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Phonon spectrum and optical properties were calculated for the orthorhombic dielectric compound of GeS. The results were obtained within the single-electron framework of density functional theory using the VASP code and generalized-gradient approximations for the exchange-correlation energy term. Phonon properties were obtained within the direct method approach which utilizes the calculated Hellmann-Feynman forces acting on atoms in a supercell. Special attention was paid to minimize errors of the calculated force constants, as the crystal is complex: it is strongly anisotropic, with two-dimensional layers having strong covalent Ge-S bonds. The interlayer coupling is, however, weak. The phonon dispersions and phonon density are in good agreement with results found in the literature. The dielectric function was also calculated and compared with available data.