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Résumé :

First-principles calculations have been performed to investigate the high pressure phase transitions and dynamical properties of the less known lead polonium compound. The calculated ground state parameters for the NaCl phase show good agreement with the experimental data. The obtained results show that the intermediate phase transition for this compound is the orthorhombic Pnma phase. The PbPo undergoes from the rocksalt to Pnma phase at 4.20 GPa. Further structural phase transition from intermediate to CsCl phase has been found at 8.5 GPa. In addition, phonon dispersion spectra were derived from linear-response to density functional theory. In particular, we show that the dynamical properties of PbPo exhibit some peculiar features compared to other III–V compounds. Finally, thermodynamics properties have been also addressed from quasiharmonic approximation.