First-principales study of the structural, vibrationa, phonon and thermodynamic properties of the complex K2PtCl6 structure hydrides Ca2OsH6

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Abstract : We have presented a full first-principles study of the structural, phonon and vibrational properties for Ca2OsH6 com-pound at the GGA-PBE level. The calculations are performed using the plane-wave pseudopotential method, density functional perturbation theory and the quasiharmonic approximation implemented in the CASTEP code. In particular, our theoretical lattice parameters obtained using the GGA-PBE to include the exchange-correlation functional are in good agreement with experiment. To our knowledge, there no experimental data or theoretical calculation for the study of frequency modes of NaCl structure of the studied hydrides for comparison.

Keywords : Hydrides, structural, phonon and vibrational properties, ab initio