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FIRST-PRINCIPLE STUDIES ON THE STRUCTURAL, ELECTRONIC AND MECHANICAL PROPERTIES OF L10 FePt

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Bimetallic FePt nanoparticles with L1₀ structure have recently gained a lot of consideration in practical applications for solid-state devices, storage of ultra-high density magnetic data and biomedicine. This is due to their high magnetic anisotropy, high magnetocrystalline anisotropy, high density, and high coercivity. These materials are also considered as nanocatalysts for growth of carbon nanotubes of different chiralities. In order gain knowledge on the structural, electronic and mechanical properties of FePt, we have carried out first-principle calculations to determine the equilibrium lattice parameters, band structure, density of states, elastic and vibrational properties 0 K. We have employed the plane-wave pseudopotential method framed within the density functional Theory (DFT) as implemented in VASP code. The Perdew–Burke–Ernzerhof (PBE) exchange-correlation functional is used with the Hubbard U-correction in the rotationally invariant form to address the self-interaction energy. The calculated equilibrium lattice parameters were found to be in good agreement with the experimental data to within 1 %, validating the approach employed. The electronic band structure and density of states have shown that FePt is metallic, due to the absence of energy band gap around the level. The bulk (209 GPa) and shear (261 GPa) moduli are relatively large, suggesting high hardness and stiffness. Finally, all elastic constants are positive and phonon dispersion curves shows no negative vibrations, suggesting mechanical stability.

Apply to be
 considered for a student
   award (Yes / No)?

No

Level for award
 (Hons, MSc,
   PhD, N/A)?

N/A

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