Density functional calculations, electronic structure, and optical properties of molybdenum bimetallic nitrides Pt_2Mo_3N and Pd_2Mo_3N

Abstract

The electronic band structure, origin of chemical bonds, and dispersion of linear optical susceptibilities for Pt_2Mo_3N and Pd_2Mo_3N have been investigated within the framework of density functional theory (DFT). The atomic positions of Pt_2Mo_3N and Pd_2Mo_3N crystalline compounds taken from the X-ray diffraction data (El-Himri, A.; Marrero-Lopez, D.; Nunez, P. J. Solid State Chem.2004, 177, 3219) were optimized by minimization of the forces acting on the atoms using a full potential linear augmented plane wave (FLAPW) method. We employed the generalized gradient approximation (GGA) of Perdew, Burke, and Ernzerhof (PBE). The DFT calculations show that these compounds have metallic origin with strong orbital hybridization near the Fermi energy level (E_F). The calculated density of states (DOS) at the Fermi energy (E_F) is about 1.83 and 1.02 states/Ry cell, and the bare linear low-temperature electronic specific heat coefficient (γ) is found to be 0.32 and 0.18 mJ/mol-K^2 for Pt_2Mo_3N and Pd_2Mo_3N, respectively. The Fermi surface of Pt_2Mo_3N (Pd_2Mo_3N) is composed of three (five) sheets. The bonding features of the compounds are analyzed using the electronic charge density contour in the (110) crystallographic plane. The linear optical properties are calculated with and without the Drude term.