SAIP2013

Contribution ID : 557

Ab initio calculations on the structural, electronic and optical properties of the hazardous silver nitrides

Friday 12 Jul 2013 at 11:30 (00h20')

Abstract :

Despite its earlier discovery, silver nitride may be the least theoretically studied compound in the late transition-metal nitrides family. The experimental characterization of silver nitride is hindered by its unstable nature. We employed first-principles calculation methods to investigate the structural, stability, electronic and optical properties of bulk crystalline Ag_3N, AgN and AgN_2 based on density functional theory (DFT) and many-body perturbation theory. The equation of state (EOS) and structural preferences for these three stoichiometries were analyzed and the equilibrium lattice parameters were determined. Bulk modulus and its pressure derivative and thermodynamic stability of all phases have been investigated. The electronic structure of the relatively most stable phases were investigated via thier band diagrams and total and orbital-projected density-of-states (DOS). Moreover, single-particle spectra of the quasi electrons and quasi holes were obtained via the GW approximation to the self-energy operator, and frequency-dependent optical constants were derived. Obtained results were comprehensively compared to previous calculations and to experimental data.Reference:* Mohammed S. H. Suleiman and Daniel P. Joubert. Theoretical calculations on the structural, electronic and optical properties of bulk silver nitrides [http://arxiv.org/abs/1212.6507]. ArXiv e-prints, December 2012.

Award :

No

Level :

PhD

Supervisor :

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Paper :

No

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Session classification : DCMPM2

Track classification : Track A - Division for Condensed Matter Physics and Materials

Type : Oral Presentation