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A Theoretical Investigation of Structural, Electronic and Optical Properties of some Group 10, 11 and 12 Transition-Metal Nitrides

By

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Abstract

Nitrides of late transition metals possess interesting properties leading to different technological applications, yet, due to many factors, synthesis and reliable characterization of the physical properties of these materials constitute a big challenge. In this work, we present a detailed firstprinciples investigation of the structural, the electronic and the optical properties of the bulk crystalline MNx (where M = Pd, Pt, Cu, Ag or Au; and x = 1/3, 1 or 2) and ZnN.

The studied structural properties include energy-volume equation of state (EOS), equilibrium lattice structural parameters, cohesive and formation energies, relative phase stabilities, bulk modulus and its pressure derivative. By means of the enthalpy-pressure EOS, some possiblepressure-induced structural phase transitions are carefully examined. Electronic properties of the energetically most stable phases are investigated via the analysis of their band structure and their total and partial densities of states (DOSs). The frequency-dependent optical constants (absorption coefficient, reflectivity, refractive index, and energy-loss spectrum) of some phases are derived from the calculated frequency-dependent microscopic dielectric tensor.

Our calculations of the structural and the electronic properties are based on density functional theory (DFT) within the projector-augmented wave (PAW) formulation and the generalised-gradient approximation (GGA) to the exchange-correlation functional. In order to improve the calculated electronic structure, and to investigate the optical spectra, we carry out expensive GW0 calculations within the the random-phase approximation (RPA) to the dielectric tensor.

Obtained results are discussed within the employed theoretical methods of calculations. Whenever possible, our obtained results are compared with experiment and with previous theoretical studies. We report the discovery of some possible low-energy competitive phases which are more stable at zero pressure than the synthesized and other hypothetical structural phases. To the best of our knowledge, our calculated optical spectra may be considered as the first, and thus, the most accurate, calculations within the many-body perturbation GWA calculations, so far.