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First-Principles Calculations of the Structural, Electronic and Optical Properties of PdN and PdN2

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Abstract content
   (Max 300 words)

The atomic and electronic structures of PdN and PdN2 were investigated using ab initio density-functional theory (DFT). We studied cohesive energy vs. volume data for a set of reported and hypothetical structures. Obtained data was fitted to a third-order Birch-Murnaghan equation of state (EOS) so as to identify the energetically most stable phases and to determine their equilibrium structural parameters. Electronic properties were investigated by calculating the band-structure and the total and partial density of states (DOS). Some possible pressure-induced structural and electronic phase transitions were tested. To derive the frequency-dependent optical spectra (i.e. absorption coefficient, reflectivity, refractive index, and energy-loss), we carried out expensive GW0 calculations within the random-phase approximation (RPA) to the dielectric tensor. Obtained results were compared with previous studies.

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

Yes

Level for award
 (Hons, MSc,
   PhD)?

PhD

Main supervisor (name and email)
and his / her institution

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Would you like to
 submit a short paper
 for the Conference
 Proceedings (Yes / No)?

Yes

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