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

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## Abstract content <br>   (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<br> consider for a student <br>   award (Yes / No)?

Yes

## Level for award<br> (Hons, MSc, <br>   PhD)?

PhD

## Main supervisor (name and email)<br>and his / her institution

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

Yes


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