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# Structural, Electronic and Optical Properties of Gold Nitrides 

Wednesday, 11 fuly 2012 16:50 (20 minutes)


#### Abstract

Max $\mathbf{3 0 0}$ words) The atomic and electronic structures of $\mathrm{AuN}, \mathrm{AuN} 2$ and Au 3 N are investigated using first-principles densityfunctional theory (DFT). We studied cohesive energy vs. volume data for a wide range of possible structures of these nitrides. Obtained data was fitted to Birch-Murnaghan third-order equation of state (EOS) so as to identify the most likely candidates for the true crystal structure in this subset of the infinite parameter space, and to determine their equilibrium structural parameters. The analysis of the electronic properties was achieved by the calculations of the band-structure and the total and partial density of states (DOS). Some possible pressure-induced structural and electronic phase transitions have been pointed out. Further, we carried out expensive GW0 calculations within the random-phase approximation (RPA) to the dielectric tensor to investigate their optical spectra. Obtained results were compared with theory and with experiment.


## 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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Session Classification: DCMPM2

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

