



Contribution ID: 557

Type: Oral Presentation

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

Friday, 12 July 2013 11:30 (20 minutes)

### Abstract content <br> &nbsp; (Max 300 words)

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  $\text{Ag}_3\text{N}$ ,  $\text{AgN}$  and  $\text{AgN}_2$  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 their 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.

### Apply to be<br> considered for a student <br> &nbsp; award (Yes / No)?

No

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

PhD

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

Daniel P. Joubert

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

No

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**Session Classification:** DCMPM2

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