Surface Electronic Structure of Gadolinium Nitride

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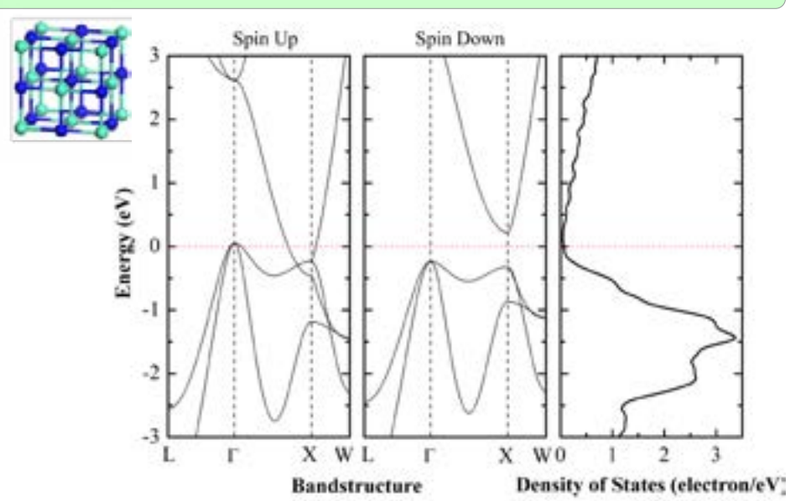
Introduction

We report our density functional theory calculations of the surface electronic structure of gadolinium nitride (GdN) (100) slabs. Our predictions of small density of states at the Fermi level and an overlap of bands at the gamma point agree well with the spectroscopy and ultraviolet photoelectron spectroscopy study of a high-quality [100]-textured GdN thin film. We also predict that GdN bulk and GdN (100) surfaces are half-metallic, which need further experimental investigations.

Methods

- Density functional theory (DFT) implemented in VASP code
- Projector augmented-wave (PAW) method
- Plane wave basis set, with energy cutoff around 400 eV
- Generalized gradient approximation (GGA) in Perdew-Burke-Ernzerhof form (PBE)
- DFT+U method with $U = 6.7$ eV and $J = 0.7$ eV for Gd
- Max force is lower than 0.02 eV/Å in optimizations.

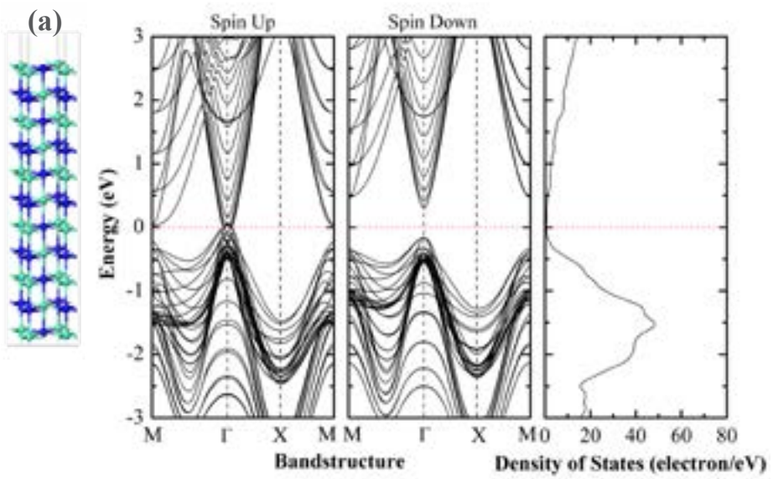
Bulk GdN

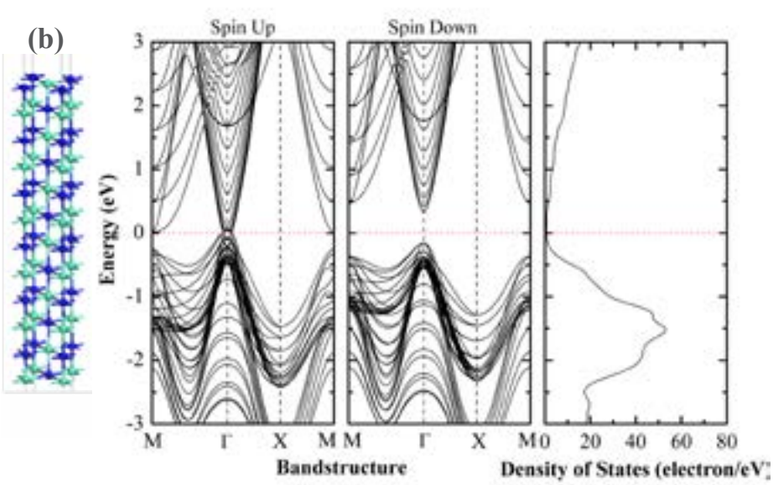


Calculated band structure and density of states for GdN bulk.

GdN (100) Slabs

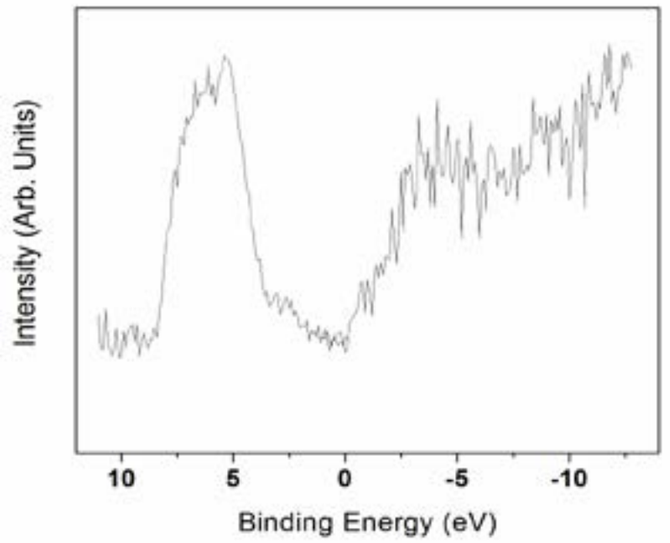
These slab models have the thickness of 11, 12, 19, and 20 unit cells with the supercells containing $Gd_{11}N_{11}$, $Gd_{12}N_{12}$, $Gd_{19}N_{19}$, and $Gd_{20}N_{20}$, respectively. Geometry optimizations for the slabs are carried out with 5 × 5 × 1 Monkhorst-Pack5 k-point grids.





Calculated band structure diagrams and density of states for (a) an 11-unit-cell thick GdN slab, (b) a 12-unit-cell thick GdN slab..

Experiments



Combined inverse photoelectron and ultraviolet photoelectron spectrum of a [100]-textured GdN thin film.

Summary

1. The densities of states for all the cases considered are very low at the Fermi level of these models.
2. Slabs of either odd or even number of layers also do not have noticeable differences in the calculated density of states.
3. Half-metallicity is predicted for GdN bulk and GdN (100) slabs by the DFT.

Acknowledgments

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