Investigating Doping Effects on the Magnetic and Energetic Nature of $Fe_{16}N_2$

Nathan Szymanski, Vijaya Adhikari, and Dr. Sanjay V. Khare

Background

Highly magnetic materials are of great importance due to their application in energy-conversion devices. Currently, the vast majority of permanent magnets contain rare-earth elements, which are limited and expensive[1].

α''- $Fe_{16}N_2$ is a promising rare-earth free magnet. It is highly magnetic, with a magnetic moment of 2.5-3.5 μ_B/Fe[2], and it consists of elements which are abundant and cheap.

However, $Fe_{16}N_2$ has a relatively low thermal stability, and is known to decay at high temperatures, which limits its level of application[3].

Goal

To identify dopants which are capable of the following:

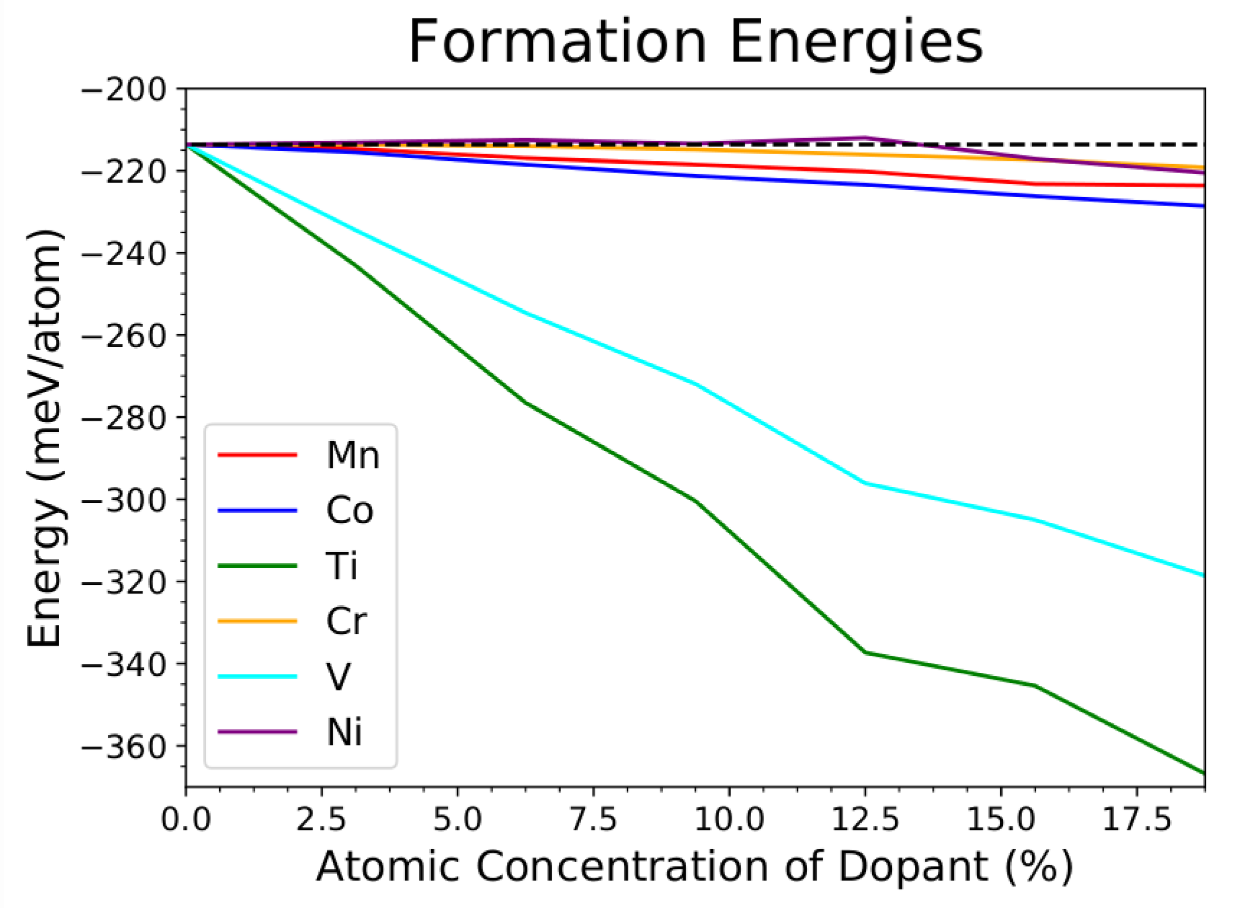
- Enhancing the thermal stability of $Fe_{16}N_2$
  Or
- Increasing the magnetic moment of $Fe_{16}N_2$

We would also like to be able to explain the physics behind the effects of each dopant.

Methods

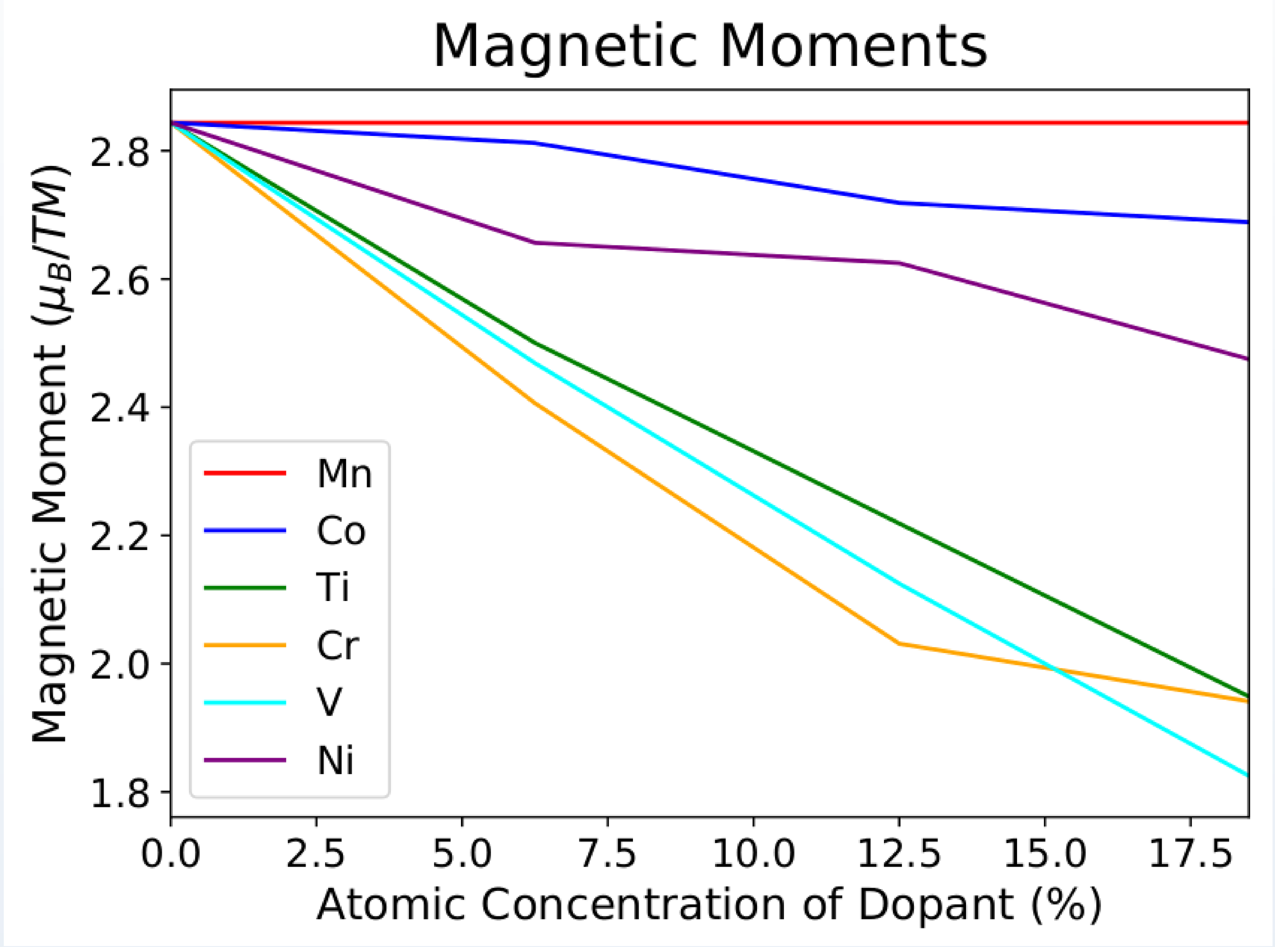
- Density Functional Theory (DFT)
  - Used to study ground state properties
  - Provides accurate prediction of structures
- Special Quasirandom Structures (SQS)
  - Allows us to simulate randomness/doping
- Hybrid Functionals (HSE06)
  - Provides accurate prediction of electronic and magnetic properties

Formation Energies



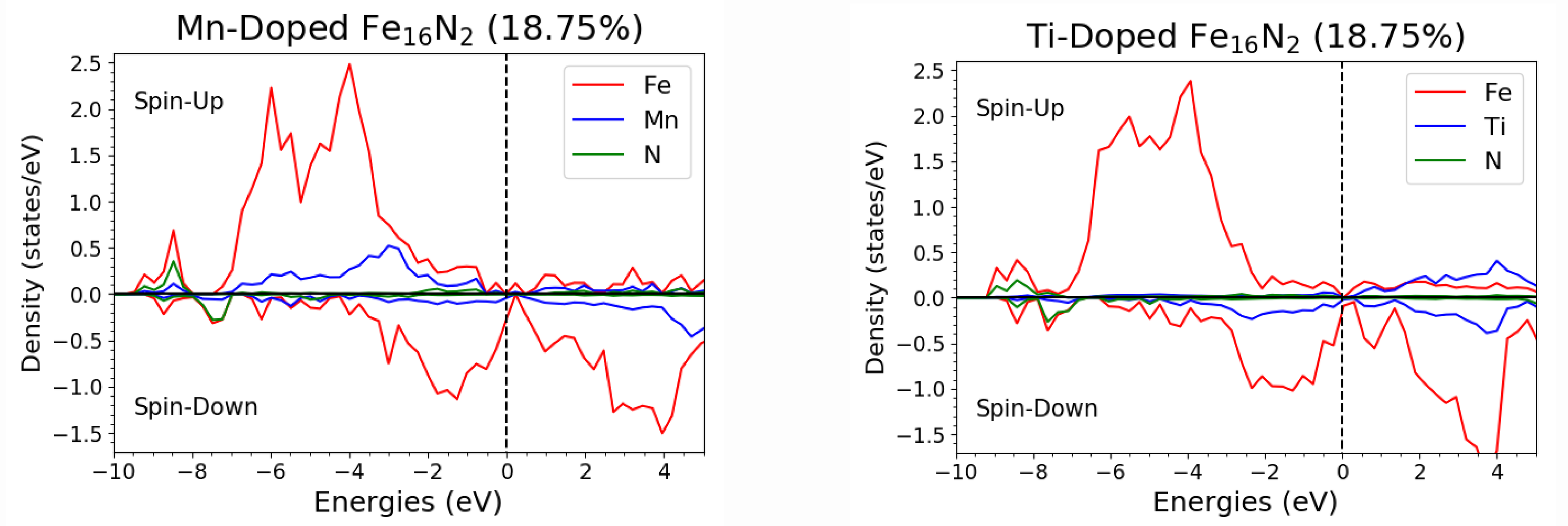
- All dopants lead to a more negative formation energy, and therefore a more stable compound.
- Ti and V are the most effective dopants to stabilize $Fe_{16}N_2$.
- Formation energy trend is mostly linear.

Magnetic Moments



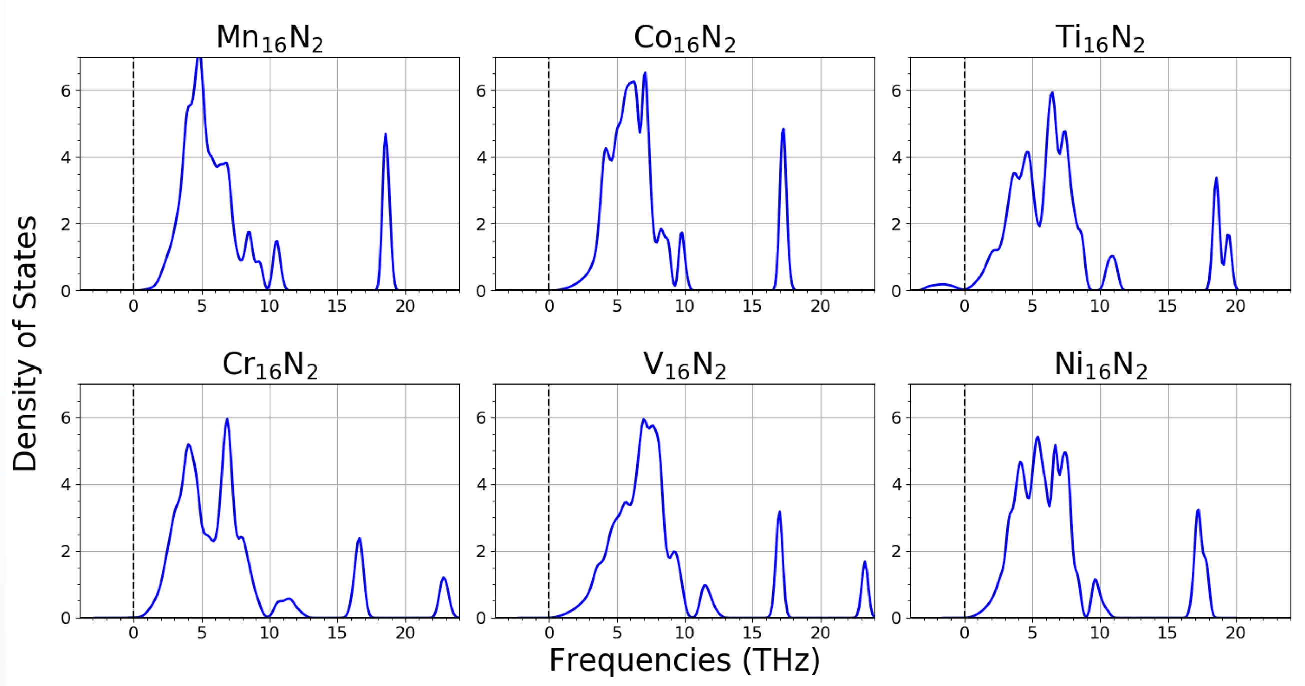
- All dopants lead to a lower magnetic moment.
- Ti, Cr, and V have the largest impact.
- Mn has almost no effect on the magnetic moment at low concentrations.

Electronic Structure



- Ferromagnetic couplers: Mn, Co, and Ni (lower impact on magnetism)
- Anti-Ferromagnetic couplers: Ti, Cr, and V (higher impact on magnetism)

End-Member Compounds



- If all phonon frequencies are positive, the compound is dynamically stable.
- All end-member compounds, except $Ti_{16}N_2$, are predicted to be stable.

Conclusion

- $Fe_{16}N_2$ is predicted to exhibit a magnetic moment of 2.82 μ_B/Fe.
- We have identified dopants which are capable of greatly enhancing thermal stability, while only slightly decreasing magnetic moment.
- Ti, Co, and V would are the most effective dopants.
- All end-member compounds (except $Ti_{16}N_2$) are predicted to be stable.

References

[1] S. Sugimoto, J. Phys. D: Appl. Phys. **44**, 064001 (2011).
[8] N. Ji, V. Lauter, X. Zhang, H. Ambaye, and J.-P. Wang, Appl. Phys. Lett. **102**, 072411 (2013).
[16] E.D.M. Van Voorthuysen, D.O. Boerma, and N.C. Chechenin, Metall. Mater. Trans. A. **33**, 2593 (2002).

COLLEGE OF NATURAL SCIENCES AND MATHEMATICS
THE UNIVERSITY OF TOLEDO
NSF