First Principles Study on the Electronic Properties of $Ca_{10}(Pt_3As_8)(Fe_2As_2)_5$

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Outline

- Motivations: Why $Ca_{10}(Pt_3As_8)(Fe_2As_2)_5$?
- Methods: Density Functional Theory (DFT)
- Results: Ground state of $Ca_{10}(Pt_3As_8)(Fe_2As_2)_5$
- Conclusions and Future Work

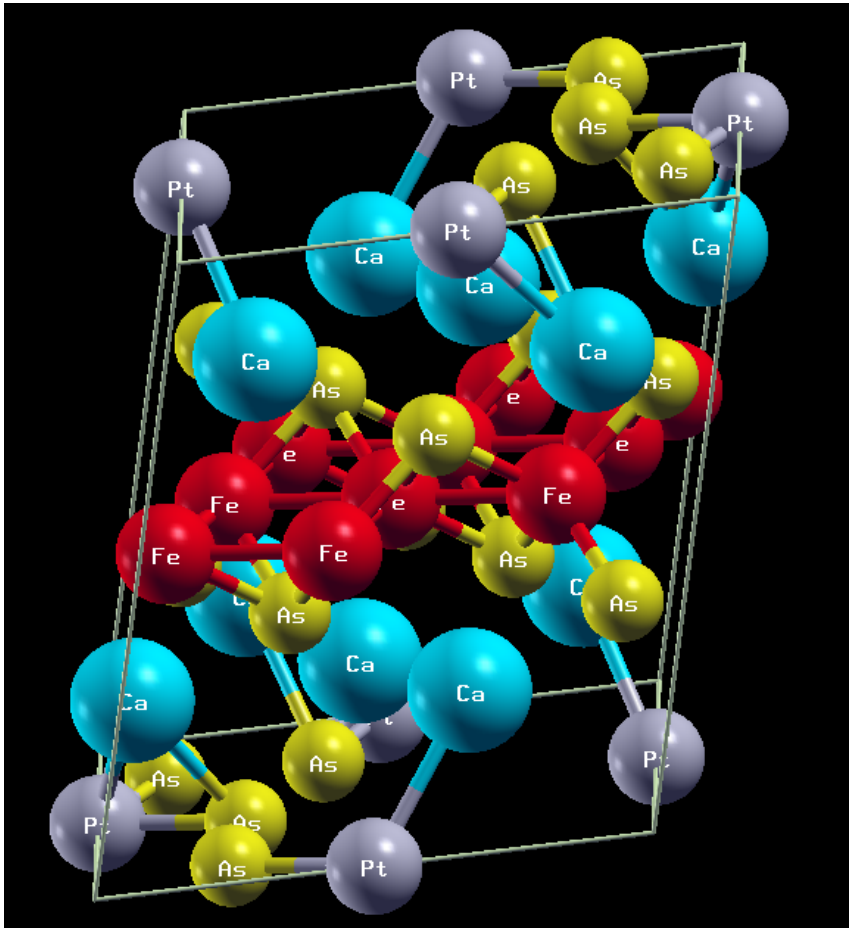
Motivations: Why $Ca_{10}(Pt_3As_8)(Fe_2As_2)_5$?

Superconductors

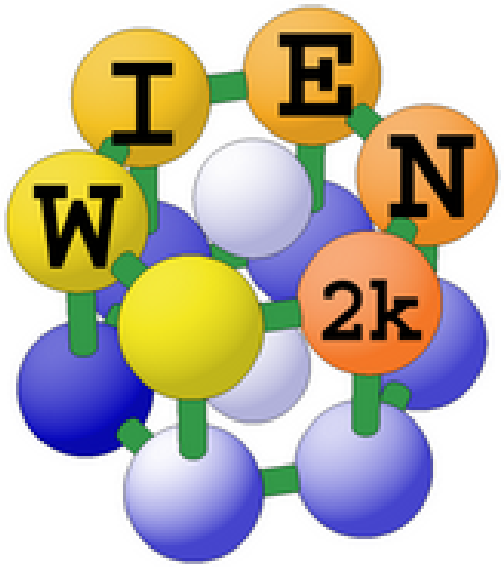
- Conduct with zero electrical resistance
- Expel magnetic fields
- Powerful electromagnets - important for technology
- Higher critical temperature of some materials still not understood

Motivations: Why $Ca_{10}(Pt_3As_8)(Fe_2As_2)_5$?

- New class: Iron-based High-T_c Superconductors
- Superconductivity could have to do with magnetic configuration
- Some research has been done, but ground state previously unknown



Methods: Density Functional Theory (DFT)



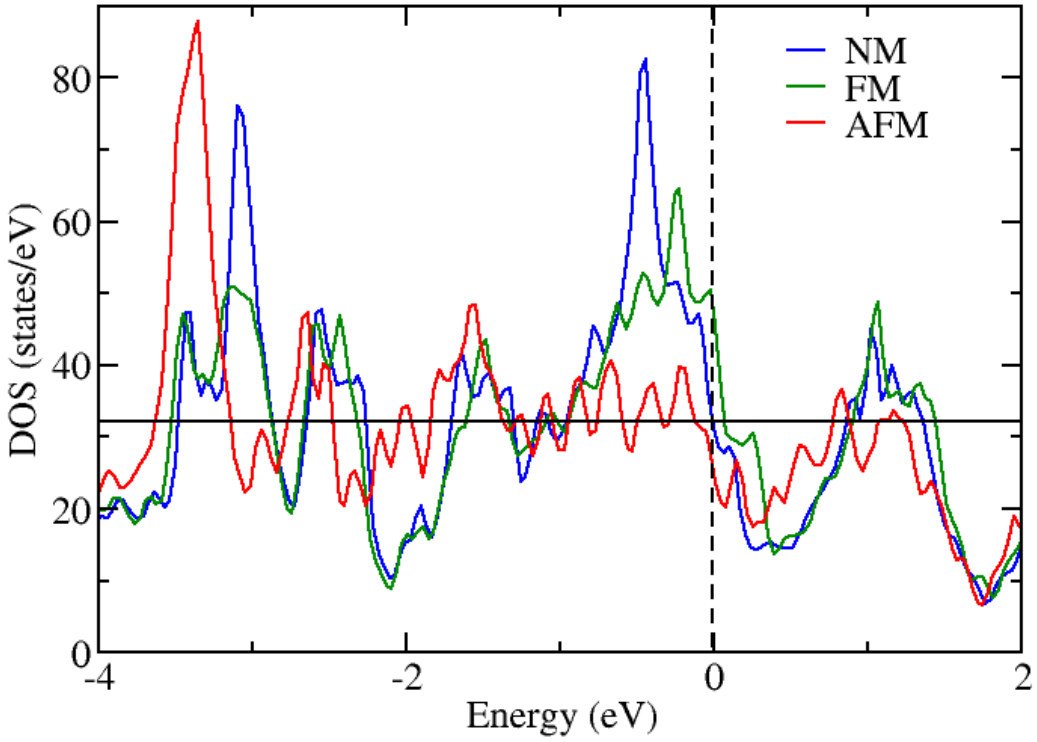
- DFT is a first-principle ab-initio method utilized in obtaining the properties of materials
- WIEN2k is an all-electron code with proven high accuracy.
- For these calculations, we ran WIEN2k on the LONI supercomputer QueenBee

Results: $Ca_{10}(Pt_3As_8)(Fe_2As_2)_5$
Ground State Energy Calculation

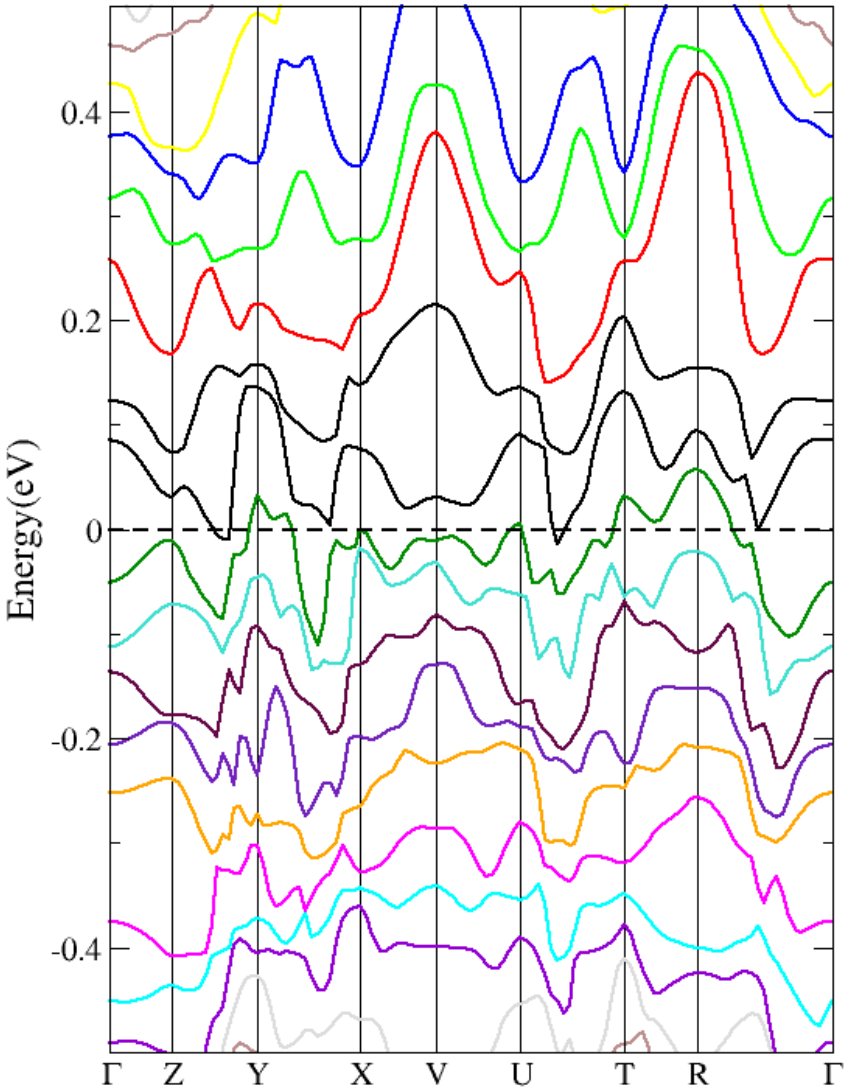
- Calculations were run for each of three magnetic configurations: nonmagnetic, ferromagnetic, and antiferromagnetic
- Lowest energy configuration: Antiferromagnetic
- Difference between antiferromagnetic energy and next level up, ferromagnetic, is 0.677 eV/Fe

Results: $Ca_{10}(Pt_3As_8)(Fe_2As_2)_5$
Density of States (DOS)

Comparison of the DOS for the nonmagnetic (NM), ferromagnetic (FM), and antiferromagnetic (AFM) configurations.



Results: $Ca_{10}(Pt_3As_8)(Fe_2As_2)_5$
Electronic Band Structure



The calculated electronic band structure in the antiferromagnetic configuration.

Conclusions and Future Work

- Antiferromagnetic ground state, followed by the ferromagnetic phase
- Importance: Doped cases can now be researched more effectively
- Fe-based superconductors could help us understand how superconductors come about

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Questions?

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