First Principles Study on the Electronic Properties of $\text{Ca}_{10}(\text{Pt}_3\text{As}_8)(\text{Fe}_2\text{As}_2)_5$

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Research Experience for Undergraduates
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 $\text{Ca}_{10}(\text{Pt}_3\text{As}_8)(\text{Fe}_2\text{As}_2)_5$?

- 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?
