Project Title: Computational Discovery and Modeling of Advanced Magnetic Materials

Project Reference Code: Chen-UAB

Name of Project Leader: Cheng-Chien Chen

Host Facility: University of Alabama at Birmingham

Internship Location: Science and Engineering Complex - East Science Hall

Host Facility Location: 902 14th Street South, Birmingham, AL 35233

Project Description (roughly 300 words):
Permanent magnets and altermagnets are two important classes of magnetic materials. Permanent magnets are critical components in modern energy technologies, including electric vehicles, wind turbines, and other energy-efficient devices. The discovery of high-performance permanent magnets, particularly those with reduced dependence on critical rare-earth elements, is essential for advancing sustainable energy technologies. Altermagnets represent an emerging class of magnetic materials that exhibit unique characteristics distinct from conventional ferromagnets and antiferromagnets. Their unconventional electronic and magnetic properties offer exciting opportunities for next-generation spintronics, magnetic memory, and information technologies. This project will focus on the computational discovery and modeling of novel permanent magnets and altermagnets. Students will investigate the relationships between crystal structures, electronic properties, and magnetic behavior, with the goal of identifying promising magnetic materials and predicting their properties.

Undergraduate students participating in this project will gain hands-on research experience in computational materials science. The research will involve first-principles density functional theory (DFT) calculations to investigate electronic structures, magnetic ordering, and material properties. Advanced quantum many-body approaches, including DFT+U and DFT combined with dynamical mean-field theory (DFT+DMFT), will be employed to study electron correlation effects. Machine learning (ML) methods will also be explored to accelerate computational searches and identify promising candidate materials. Students will receive training in computational materials modeling, Python programming, Linux shell scripting, and high-performance computing. They will participate in different aspects of the research, ranging from computational simulations and data analysis to ML-assisted materials discovery. In addition, students will develop scientific communication and writing skills through regular research discussions, presentations, and preparation of research reports and manuscripts.

Disciplines:
Physics, Computer Science, and Materials Science.

Importance:
The discovery of advanced permanent magnets and altermagnets could enable the development of more efficient electric vehicle motors and wind turbines with reduced reliance on critical rare-earth elements, as well as next-generation spintronic devices and magnetic memory technologies with faster operation, lower energy consumption, and higher information storage density.

Requirements:

- Preferred Major
  - Physics, Chemistry, Math, Computer Science, and Materials Science.
- Class work
  - NA
- Programming knowledge
  - Python programming, Linux shell scripting.
- Software knowledge
  - NA
- Other

Biography (roughly 100-150 words):

Prof. Cheng-Chien Chen's research focuses on computational materials modeling, using first-principles calculations, quantum many-body techniques, and machine learning simulations. He received his PhD in Physics from Stanford University in 2011. He subsequently served as a Postdoctoral Scholar at SLAC National Accelerator Laboratory and as an Aneesur Rahman Postdoctoral Fellow at Argonne National Laboratory. He joined the Department of Physics at the University of Alabama at Birmingham (UAB) in 2016. His research has been funded by the U.S. Department of Energy, the Air Force Office of Scientific Research, and the National Science Foundation (NSF), including an NSF CAREER Award.

Is U.S. citizenship required to participate in this project? No

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