

Invited Seminar

A (Spin) Polarized World: Multiscale Modelling of Magnetic Materials for Energy Applications

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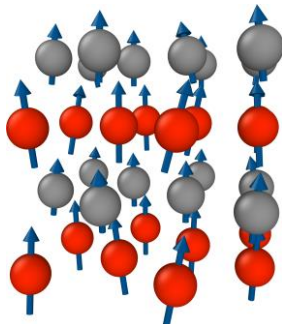
Hosts: Dr. Criss Zhang (xiao.zhang@northeastern.edu), Prof. Laura H. Lewis

April 18th, 2024

11 am – 12 pm (ET)

Location: SN 358

Abstract: Magnetic materials surround us in our everyday lives. Examples range from the magnetically ‘soft’ core of an electrical transformer to the permanent magnets used in a modern electric motor, all the way down to the magnetic oxides used as recording materials in hard disc drives. Deepening our understanding of fundamental physics and giving these materials their desirable properties has the potential to enable the development of improved materials for both new and existing applications. In addition, amid a global ‘critical materials’ crisis, there is a growing desire to discover sustainable alternatives to some of the established magnetic materials, reducing pressure on global raw-materials reserves.



The ferromagnetic state of $L1_0$ FeNi

In this talk, I will elucidate the crucial role of theory and computational modeling in developing our understanding of magnetic materials and optimizing their physical properties for applications. The focus will be on materials modeling at the atomic length scale using density functional theory (DFT) calculations and interatomic potentials. I will demonstrate how the magnetic state of an alloy can affect how atoms prefer to arrange themselves [1], how these atomic arrangements can influence a material’s magnetic properties [2], and also give examples of how machine learning can accelerate the materials modeling process [3].

References:

- [1] Woodgate, Hedlund, Lewis, Staunton, *Phys. Rev. Materials* **7**, 053801 (2023).
- [2] Woodgate, Patrick, Lewis, Staunton, *J. Appl. Phys.* **135**, 163905 (2023).
- [3] Shenoy, Woodgate, Staunton, et al., *Phys. Rev. Materials* **8**, 033804 (2024).

Biography: Chris earned his Ph.D. from the University of Warwick (UK), where he currently serves as a Research Fellow in the Department of Physics. His research focuses on computational modeling of the physics of alloys and magnetic systems, with extensive interdisciplinary collaboration. Outside of research, Chris finds time to practice the sport of archery and the hobby of English-style change ringing.

