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Design Principles for Materials with Magnetic Functionality



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Design Principles for Materials with Magnetic Functionality

Principles allow development of technically useful magnetic materials devoid of rare-earth elements

BACKGROUND & MOTIVATION

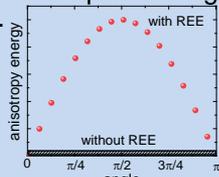
The DOE Critical Materials Strategy identifies a national need for useful magnetic materials free of expensive rare-earth elements (REE). Without these elements, useful magnets require extensive processing.



INNOVATION

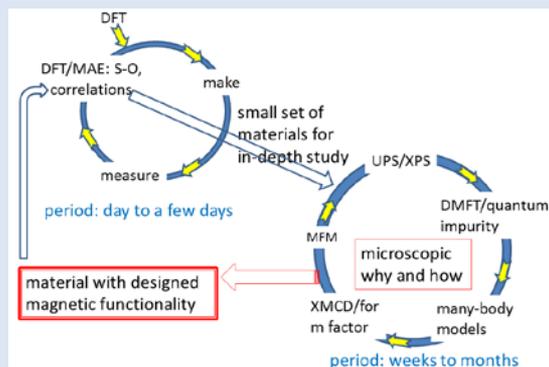
Experimentally validated theoretically predicted design principles for REE-free materials whose intrinsic magnetic properties equal or exceed those presently requiring extensive processing

- Useful magnet materials require strong magnetic anisotropy.
- Anisotropy is not intrinsic to most materials without rare-earth elements.
- New scientific principles and novel 1st principles theory (Dynamic Mean Field Theory - DMFT) were developed to predict anisotropy in REE-free materials.



DESCRIPTION

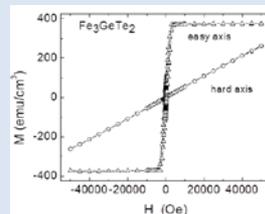
Developing necessary scientific design principles requires closely integrated efforts in theory, modelling, synthesis, and measuring.



Iteratively closing these two loops has yielded new design principles:

- Need intrinsic structural anisotropy (hexagonal or tetragonal most desirable)
- Need a high density of magnetic elements such as iron or cobalt
- Need strong electron-electron correlations
- Desirable to have a heavy transition metal to augment spin-orbit interactions

Demonstrated design principles in Fe₃GeTe₂



Current Technology Readiness Level (TRL) 1

- Basic scientific principles are being refined and tested.

ANTICIPATED IMPACT

Approach to developing design principles for materials with desired functions is broadly applicable to 'materials-by-design' needs of the Laboratory and Nation.

- Principles from atomic to macroscopic length scales
- Concepts applicable to developing principles for designing emergent function in materials with applications to sensing, actuating, and computing
- Strategic magnetic materials containing inexpensive transition metals

PATH FORWARD

Development steps

- Speed up DMFT calculations
- Open source codes for calculating electronic structures of complex materials
- Explore composition-space of relevant compounds. Characterize optimal materials.

Potential End Users:

- DOE-OS, EERE (critical materials), DARPA
- Electronics, magnetic storage, wind, quantum device industries

Point of Contact: Joe D. Thompson,
MPA, 7-6416, jdt@lanl.gov