Title: Solid-state Magnetic Refrigeration: First-principles Modeling and Computational Materials Search

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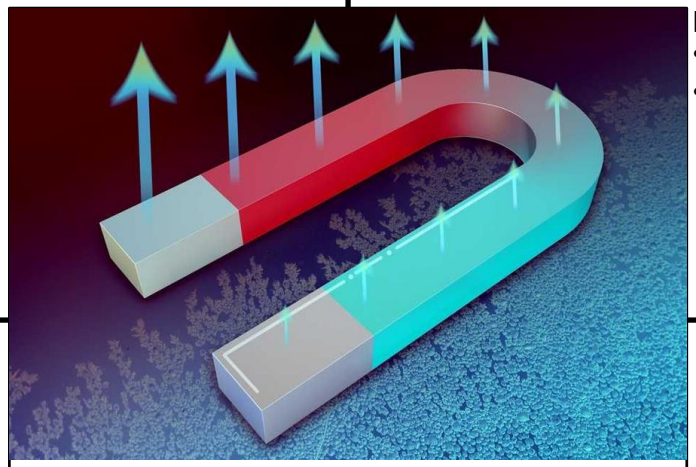
Research Objectives

- Develop first-principles simulation methods to directly predict ADR refrigerant performance, novel solid-state heat switches, and alternative continuous magnetic refrigeration.
- **Innovation:** new computational method, novel heat switch mechanism, new concept for continuous magnetic refrigeration
- **SOA:** no first-principles methods exist for ADR; no ADR refrigerant in 10-30K; heat switches involving gas and moving parts; multistage ADR for continuous operation
- **Start TRL**: 2; **End TRL**: 3
- **TRL justification:** ADR and MFC concept already exist. No systematic modeling methods exist for ADR; no efficient ADR refrigerant exist for 10 to 30K; no detailed understanding of MFC and promising material candidate.



A schematic of solid-state continuous magnon flow cooling: pumping heat by a non-uniform magnetic field

Approach

- Modeling magnon, electronic and phonon thermal and transport properties using DFT, spin-DFT, atomistic spin dynamics simulation and Boltzmann equation solver
- High throughput computational materials search for novel ADR refrigerants in 10 to 30 K.
- Simulation phonon transport in ferroelectric oxides under an external electric field for heat switching application
- Solving coupled magnon-phonon Boltzmann transport equations to understand the continuous MFC mechanism and suggest promising candidate materials for MFC implementation

Potential Impact

- New ADR refrigerants to enable efficient solid state magnetic refrigeration in the temperature range of 10 to 30 K
- New methods to predict ADR performance from first-principles
- New solid-state heat switches to replace existing gas gap (with gas leakage risk), mechanical (with moving parts), and superconducting (inefficient > 10 K) heat switches for ADRs
- New continuous magnetic refrigeration mode to replace multistage ADRs (highly complex in design and operation)
- **our project will lead to more efficient, reliable, compact and cost-effective solid state cooling technologies for space missions that can operate at different temperature ranges.**