Hessisches Kompetenzzentrum
für Hochleistungsrechnen

High-Throughput Calculating of Magnetic Ground State

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Project Term
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Clusters
Lichtenberg II Cluster Darmstadt

Software
VASP, VAMPIRE

Additional Software
FPLO, TB2J, Wannier90

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Introduction

Magnetic materials are at the heart of modern technologies ranging from information storage to next-generation spin-based electronics. A central scientific problem is to determine the magnetic ground state of a material, meaning the most stable arrangement of atomic magnetic moments. This state governs many important properties such as electrical transport, heat flow carried by magnetic excitations, and novel quantum effects. Recently, a new class of materials has emerged that combines features of different types of magnets and shows unusual electronic and magnetic behavior. Understanding these systems requires precise knowledge of how magnetic moments on different atoms interact with each other. The challenge is that such interactions depend sensitively on crystal structure, chemical composition, and relativistic effects. For realistic materials, they cannot be obtained analytically and must be computed from quantum-mechanical simulations. Because thousands of candidate magnetic materials are now available in crystallographic databases, a systematic exploration becomes a large-scale problem. Each material requires many separate calculations under different magnetic configurations, which makes the project ideally suited for high-performance computing. The present project therefore uses automated large-scale simulations to determine magnetic ground states and related properties across a broad materials set.

Methods

We employ first-principles quantum-mechanical simulations to describe the electronic structure of solids without adjustable

parameters. For each material, we compute total energies for several distinct magnetic configurations. By comparing these energies, we extract effective interaction parameters between atomic magnetic moments. These parameters form the basis of a simplified model that captures the essential magnetic physics of the system. To ensure reliability, we use two complementary approaches. One is based on direct comparison of total energies of different spin arrangements. The other uses a Green's-function technique derived from the electronic structure in a localized orbital representation. This second approach requires the construction of Wannier functions, which allow efficient interpolation of electronic properties on extremely dense momentum grids. Once the interaction parameters are known, we determine the magnetic ground state and compute magnetic excitation spectra. From these excitations, we evaluate how heat and charge transport are influenced by magnetism. The entire procedure is embedded in an automated workflow that handles structure preparation, job submission, error correction, and data analysis, enabling high-throughput treatment of thousands of materials.

Results

During the reporting period, we established a fully automated workflow that links electronic-structure calculations, Wannier function construction, and magnetic-interaction analysis. This infrastructure allows large numbers of materials to be treated in a consistent and reproducible manner. We validated the workflow using well-known magnetic systems, where computed interaction strengths and excitation spectra agree with experimental and literature data. Using this framework, we completed magnetic-interaction calculations for roughly 900 materials from the magnetic materials database. For these systems, we determined the range and strength of interactions between magnetic atoms and constructed effective models describing their magnetic behavior. Preliminary magnetic excitation spectra were obtained for representative materials, confirming that the derived models are physically meaningful. In addition, we screened the database for materials with symmetry properties suggesting unconventional magnetic behavior. Several promising candidates were identified and analyzed in more detail, revealing characteristic features in their electronic structures. These findings demonstrate that large-scale computational screening can successfully uncover materials with unusual magnetic and transport properties.

Discussion

The project demonstrates that automated high-throughput simulations are a powerful tool for mapping magnetic interactions across a vast materials space. The main computational difficulty lies in the enormous number of calculations required. Each material must be studied in multiple magnetic configurations, often including relativistic effects, and high accuracy demands dense sampling of the electronic structure. Furthermore, the construction of Wannier functions and evaluation of magnetic excitation properties add additional

computational steps. Altogether, these tasks generate millions of core hours of demand, which makes high-performance computing indispensable. The results so far establish a growing database of magnetic interaction parameters and ground-state predictions. This provides a foundation for understanding how crystal symmetry and electronic structure control magnetic order and related transport phenomena. In the next phase, we will extend calculations to the remaining materials, refine excitation spectra, and systematically analyze the link between magnetic symmetry and transport behavior. The project thus contributes both methodological advances in large-scale magnetic simulations and new insight into emerging magnetic materials.

Publications

Zhu, Yuhan, et al. "Metallic tellurium for p-type contacts of two-dimensional MoTe2 field-effect transistors." Nature Communications (2026). https://dx.doi.org/10.1038/s41467-025-67948-2

Li, Fu, et al. "High-Throughput Screening of Spin Hall Conductivity in Two-dimensional Materials." Nano Letters (2026). https://dx.doi.org/10.1021/acs.nanolett.5c06229

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