PHD PROJECT DESCRIPTION
(4000 characters max., including the aims and work plan to be published online)

Project title: Multiscale modelling of thermal transport in magnetic kagome materials

1.1. Project goals

The development of efficient thermoelectric materials requires the simultaneous optimization of electronic transport and suppression of lattice thermal conductivity [1]. In magnetic topological materials, such as kagome transition-metal compounds, this challenge is particularly compelling due to the interplay between electronic topology, magnetism, and lattice dynamics [2]. While recent studies have highlighted the potential of these systems for transverse thermoelectric applications, a systematic understanding of how their thermoelectric properties can be controlled and optimized is still lacking [2]. The central goal of this PhD project is to investigate and control lattice thermal transport in selected kagome materials using a combination of first-principles calculations and machine-learning-based atomistic modelling. Particular emphasis will be placed on understanding the role of chemical substitution, disorder, and defects in phonon scattering and thermal conductivity [3]. The project will be carried out in collaboration with international partners in China with expertise in machine-learning potentials and large-scale simulations.

1.2. Outline

The project will focus on a class of transition-metal compounds with kagome structures, selected from prior high-throughput screening. Examples of relevant material families include ferromagnetic materials such as Fe_3Sn and Fe_3Sn_2 as well as noncollinear antiferromagnetic kagome compounds such as Mn_3Sn and Mn_3Ge [4,5,6]. The research will combine density functional theory (DFT) calculations with advanced modelling techniques to describe lattice dynamics and thermal transport. Initially, the candidate will compute phonon spectra and lattice thermal conductivity of selected pristine systems using first-principles methods combined with semiclassical transport modelling based on the phonon Boltzmann transport equation. Subsequently, the effects of alloying, vacancies, and other defects will be investigated to identify mechanisms leading to a reduced thermal conductivity. Given the computational limitations of direct DFT approaches for complex disordered systems, machine-learning interatomic potentials will be developed and employed to enable large-scale molecular dynamics simulations [7]. These simulations will enable a detailed analysis of phonon scattering processes induced by chemical disorder and structural imperfections. The results will be used to establish design principles for engineering low thermal conductivity in these materials. The project will be closely linked to ongoing experimental and theoretical efforts within an international collaborative framework.

1.3. Work plan

The doctoral project is planned over four years. Key responsibilities will include:

1. Performing first-principles calculations of lattice dynamics in selected kagome materials;
2. Modelling lattice thermal conductivity via the phonon Boltzmann transport equation;
3. Performing electronic structure calculations including defects, alloying, and disorder;
4. Constructing machine-learning interatomic potentials from these calculations;
5. Carrying out large-scale molecular dynamics simulations to study thermal transport;
6. Collaborating with international partners and contributing to joint research activities;

7. Preparing scientific reports and manuscripts under the guidance of the supervisors;
8. Presenting research results at international conferences and in peer-reviewed journals.

Additional responsibilities may be assigned during the course of the research project, depending on the evolving scientific context and the candidate's doctoral progress. These changes will be at the reasonable discretion of the supervisors.

1.4. Literature (max. 7 listed as a suggestion for a PhD candidate preliminary study)

[1] P. Baskarana and M. Rajasekar, RSC Advances **14**, 21706 (2024)
[2] Q. Wang, *et al.,* Accounts of Materials Research **5**, 786 (2024)
[3] C. Wu, *et al.,* ACS Nano **18**, 31660 (2024)
[4] T. Chen, *et al.,* Science Advances **8**, eabk1480 (2022)
[5] M. Ikhlas, *et al.,* Nature Physics **13**, 1085 (2017)
[6] T. Chen, *et al.,* Nature Communications **12**, 572 (2021)
[7] M. Yazdani-Kachoei, *et al.*, preprint at arXiv:2412.10794

1.5. Required initial knowledge and skills of the PhD candidate

The successful candidate should hold a Master's degree in Condensed Matter Physics, Materials Physics, Theoretical Chemistry, or a closely related field, with excellent academic performance. A solid understanding of quantum mechanics, solid-state physics and basic electronic structure theory is required. Prior experience with electronic structure codes is required. Research projects and theses focused on electronic structure calculations will be considered an asset. Scientific publications are not mandatory, but will be regarded as a plus if of high quality. The ability to communicate in English is required, while proficiency may be considered an advantage. The candidate should be able to work both independently and as part of a research team.

1.6. Expected development of the PhD candidate's knowledge and skills

By the end of the PhD project, the candidate will be expected to have acquired:

1. A solid knowledge of condensed matter theory and materials physics;
2. A good knowledge of first-principles theories for electronic structure calculations;
3. A good knowledge of multiscale methods and machine-learning techniques for lattice dynamics;
4. A basic knowledge of magnetism, topology and strongly correlated materials.

Skills developed by the PhD candidate will include:

1. Proficiency with DFT calculations;
2. Proficiency in scientific programming and high-performance computing;
3. Strong analytical and problem-solving abilities;
4. Basic expertise with multiscale modelling of magnetic systems;
5. Experience in writing scientific papers and presenting research at international meetings;
6. Collaborative skills through international research interactions.