

1. PHD PROJECT DESCRIPTION (4000 characters max., including the aims and work plan)

Project title: Complex magnetism in rare earth systems

1.1 Project goals

Rare-earth elements have a crucial importance in modern society, since they are common components in industrial permanent magnets and therefore play a key role in the rise of the green technology. Despite their importance in magnetism, the electronic and magnetic properties of rare-earth compounds are still not well understood, due to the difficulties in providing an accurate description of both localized 4f states and itinerant spd states [1]. The central goal of this PhD project is to employ state-of-the-art electronic structure theory to investigate the magnetic properties of rare-earth-based systems of various types. A primary aspect to investigate will be the role played by the anisotropic terms of the exchange, including both the inter- and intra-atomic coupling. Collaboration and scientific exchange with foreign universities in the Netherlands and Sweden is expected, and further opportunities may arise during the project.

1.2 Outline

The research will be structured around a comparative analysis of various systems containing rare-earth elements, including for example rare-earth adatoms on graphene, rare-earth adatoms on magnesium oxide, and elemental rare-earth metals. This variety of systems will cover different degrees of hybridization between the rare-earth atoms and their effective medium as well as a change of the local crystal field, making it possible to have an instructing comparison between the predicted physical properties and the available experimental data. The electronic structure problem will be addressed via density functional theory (DFT) [2] and its combination with dynamical mean-field theory (DFT+DMFT) [3]. Implementations of these techniques in the RSPt code [4] and the TRIQS library [5] will be used, as they are both available as free software. These tools will allow for an accurate description of the strong electronic correlations characterizing the 4f electrons, which were previously shown to be essential to predict cohesive and spectroscopic properties [1]. The analysis of the intra-atomic exchange coupling will be conducted by means of an in-house developed code [6], which the candidate is supposed to improve and extend during the course of the doctoral studies. Eventually, depending on the interest and skills shown by candidate throughout the project, multiscale modeling for magnetism will be performed by constructing effective Heisenberg Hamiltonians to be solved via atomistic spin dynamics (ASD) [7]. The planned research will involve international collaborations with Uppsala University, Sweden, and Radboud University Nijmegen, the Netherlands, especially in relation to the construction of model Hamiltonians.

1.3 Work plan

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

1. employing ab-initio electronic structure theory to determine the intra-atomic exchange coupling in selected systems containing rare-earth elements;
2. contributing to theoretical developments, software implementation, or numerical simulations, depending on the candidate's background and proclivities;
3. actively collaborating with other project members and international partners;
4. preparing scientific reports and drafting manuscripts under the guidance of the supervisors and collaborators;
5. disseminating research results through journal articles and conference presentations.

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. 10 listed, as a suggestion for a PhD candidate)

- [1] I. L. M. Locht *et al.*, Physical Review B **94**, 085137 (2016)
- [2] R. M. Martin, *Electronic Structure*, Cambridge University Press (2004)
- [3] G. Kotliar and D. Vollhardt, Physics Today **57**, 53 (2004)
- [4] J. Wills *et al.*, Full-Potential Electronic Structure Method, Springer Berlin-Heidelberg (2010)
- [5] O. Parcollet *et al.*, Comp. Phys. Comm. **196**, 398 (2015)
- [6] M. Pivetta *et al.*, Physical Review X **10**, 031054 (2020)
- [7] C. Etz *et al.*, Journal of Physics: Condensed Matter **27**, 243202 (2015)

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 an advantage, particularly with all-electron codes. Research projects and theses focused on electronic structure calculations, statistical physics, or many-body physics 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 quantum theory of magnetism;
2. A good knowledge of first-principles theories for electronic structure calculations;
3. A good knowledge of many-body methods to describe strongly correlated materials;
4. A basic knowledge of multiscale methods for magnetism and materials design.

Skills developed by the PhD candidate will include:

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