Master 2: International Centre for Fundamental Physics

INTERNSHIP PROPOSAL

Laboratory name: CPHT CNRS identification code: UMR 7644
Internship director: Leonid Poyurovskiy
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Internship location: Ecole Polytechnique and Collège de France
Thesis possibility after internship: YES
Funding: NO (need to apply to a scholarship)

Ab initio theory of magnetic order in rare-earth intermetallics

Magnetic intermetallics containing rare-earth elements play an important role in modern industry and sustainable energy production. In particular, rare-earth-based magnetocaloric materials for cryogenic magnetic refrigeration have attracted recently a lot of attention. These materials exhibit magnetic orders due to 4f quasi-atomic shells of rare-earth coupled by inter-site exchange. The intersite exchange (IE) interaction between 4f shells can be provided through the on-site Hund's rule exchange between the 4f moment and itinerant electrons; alternatively, it may be also induced by 4f hybridization with those itinerant states. The rare-earth 4f shells are also impacted by crystal electric field (CEF) induced by crystalline environment. All these coupling constants - various IE processes and CEF - typically have comparable magnitudes; their subtle interplay results in complex magnetic orders of rare-earth intermetallics. Current understanding of the relative importance of various coupling mechanisms and the ability to predict the actual magnetic orders in these systems are still rather limited.

The goal of this internship will be to carry out ab initio analysis of a selected set of compounds from the $R\mathrm{Co}_2$ and $R\mathrm{Cu}_2X_2$ families of rare-earth intermetallics (where R is a rare-earth ion, X is Si or Ge) with the aim of establishing the role and relative importance of various coupling mechanisms and CEF in their magnetic orders. The project will be based on methodologies developed in the CPHT Condensed matter theory group for calculating CEF potentials [1] and IE interactions [2]. These approaches are based on the DFT and dynamical mean-field theory as well as a quasi-atomic approximation for 4f shells; they have been previously successfully used to investigate rare-earth-based hard magnets [3-5] and exotic magnetic orders in f-electron insulators [6,7].

[1] P. Delange, S. Biermann, T. Miyake, and L. Pourovskii, Phys. Rev. B **96**, 155132 (2017).
[2] L. V. Pourovskii, Phys. Rev. B **94**, 115117 (2016).
[2] L. Pourovskii et al., Phys. Rev. B **101**, 214433 (2020).
[3] A. Galler et al., npj Quantum Materials **6**, 2 (2021).
[5] J. Boust et al., Phys. Rev. Materials **6**, 084410 (2022).
[6] L. V. Pourovskii and S. Khmelevskyi, PNAS **118**, e2025317118 (2021).
[7] S. Khmelevskyi and L. V. Pourovskii, Communications Physics **7**, 12 (2024).

Please, indicate which speciality(ies) seem(s) to be more adapted to the subject:

Condensed Matter Physics: YES Soft Matter and Biological Physics: NO
Quantum Physics: YES Theoretical Physics: YES