Magnetic order at surfaces beyond the Heisenberg model

Spin structures at surfaces driven by higher-order exchange interactions

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In Short

- Higher-order exchange interactions beyond pair wise Heisenberg exchange can play an important role for magnetism at surfaces.
- Novel spin structures can occur which are interesting with respect to hybrid structures with superconductors or as the origin of topological orbital magnetization.
- We use density functional theory in combination with atomistic spin models to explore the effect of higher-order exchange interactions for ultrathin films studied experimentally by our collaborators via spin-polarized scanning tunneling microscopy.

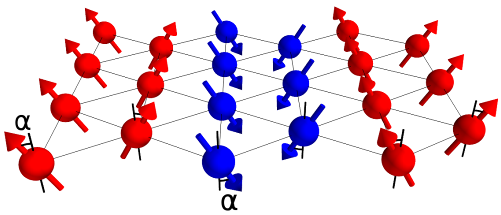

***Figure 1:** Canted ↑↑↓↓ state within a monolayer thick magnetic film due to the competition of higher-order exchange interactions and the Dzyaloshinskii-Moriya interaction. Blue and red spheres and arrows denote the atoms and spin directions, respectively, within the hexagonal monolayer. This novel spin structure was discovered in an atomic Fe/Rh bilayer on Ir(111) using spin-polarized scanning tunneling microscopy and explained based on density functional theory calculations [6].*

The magnetic ground state of a material is governed by the magnetic interactions between atomic magnetic moments. In addition to the Heisenberg pairwise exchange interactions also higher-order exchange interactions can play a role, where exchange between more than two sites is involved [1]. In complex three-dimensional spin structures on the nanometer scale such interactions can be the decisive factor for the magnetic ground state. While several spin structures at surfaces stabilized by higher-order terms are known [2],[3],[4],[5],[6] the understanding of these interactions is still very limited. Recently, an additional higher-order exchange interaction was proposed theoretically [5] in order to understand discrepancies between results from density functional theory (DFT) and previously used atomistic spin models [7]. A realistic spin model, that describes the magnetic interactions accurately, is indispensable for further investigations regarding predictions for materials with tailored properties, such as magnetic ground state, phase transitions, thermodynamical stability, and spin dynamics.

In this project we aim to gain more insight into the role of higher-order interactions in atomically thin magnetic layers on single crystal surfaces. Such systems can serve as model systems to understand the microscopic origin of complex magnetic order and the involved interactions. In our approach we combine DFT calculations and atomistic spin dynamics simulations. We collaborate with the experimental group of Prof. R. Wiesendanger, in particular, with Dr. Kirsten von Bergmann who is an expert in spin-polarized scanning tunneling microscopy. Several ultrathin film systems will be studied and we expect to discover novel types of spin structures. In addition we would like to explore whether higher-order exchange interactions can modify the properties of topological spin structures such as skyrmions or antiskyrmions.

We will use DFT calculations to obtain total energies for a variety of collinear and noncollinear spin structures. From these calculations we can parametrize an atomistic spin model including pairwise Heisenberg exchange, the Dzyaloshinskii-Moriya interaction as well as higher-order terms such as the biquadratic and the four-spin interaction. Spin dynamics simulations using our in-house developed code (as e.g. in [8]) will be applied to find new magnetic ground states based on this DFT parametrized atomistic spin model and to explore the properties of skyrmions in systems with significant higher-order terms. We will study model systems in order to understand the trends of the magnetic interactions as well as ultrathin films on surfaces which can be directly compared to the experimentally studied systems.

Our goal is to discover novel spin structures driven by higher-order exchange interactions, to identify their origin and to establish a suitable atomistic spin model. We anticipate that the fundamental understanding of the role and occurrence of higher-order interactions obtained here will also be relevant beyond complex magnetic ground states in monolayers, e.g. in the context of hybrid systems where non-collinear magnetic order is in contact with superconductors or is the source of topological orbital magnetization [9],[10].

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http://www.itap.uni-kiel.de/theo-physik/heinze/

More Information

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Project Partners

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