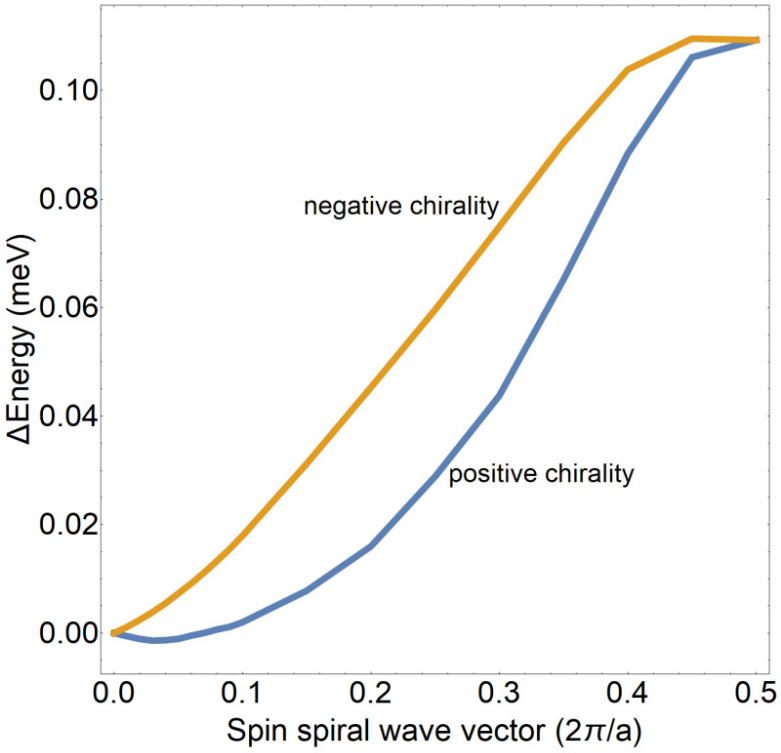
Electronic Theory of the Magnetic Order in Thin Films



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2023 - 2024

Clusters
Lichtenberg II Cluster Darmstadt

Software
VASP

Institute
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University
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Introduction

Symmetry, dimensionality, and local environment are essential elements affecting the magnetism of transition-metal systems. Over the past decades, extensive research in this area has uncovered numerous fundamentalnew phenomena, some of which have lead to significant technological advancements. Typical for low-dimensional magnetic systems is the occurence of noncollinear magnetic order, which involves the interplay between isotropic, anisotropic, symmetric and antisymmetric exchange interactions between local magnetic moments. Of particular interest in this context is the antisymmetric exchange, which is a consequence of spin-orbit coupling, as it favors noncollinear magnetic orders with precise local chiralities resulting in the formation of spiral magnetic order and vortex magnetic patterns known as skyrmions. The main goal of this project is to develop a microscopic understanding of the antisymmetric exchange and its consequences on the equilibrium and dynamic properties of transition-metal thin films. Since the antisymmetric exchange is a consequence of spin-orbit coupling, quantum mechanical many-electron calculations are needed to quantify it. These calculations are very costly in terms of computing time and thus are only feasible in combination with high performance computing centres such as the NHR4CES.

Methods

The results were obtained by using density functional theory (DFT), which is a quantum mechanical method for determining the ground state of many-electron systems. In contrast to other methods such as Hartree-Fock, DFT works with the electron density, which only depends on the three spatial coordinates. Consequently, DFT requires considerably less computing power, which allows us to perform calculations involving hundreds of atoms in modern high-performance computing architectures, which enables calculations such as the ones performed in this project.

Results

In the framework of density functional theory, the frozen-magnon dispersion relations of FePt and CoPt bilayers have been calculated. Moreover, the parameters of the associated generalized Heisenberg models have been extracted. It is shown that spin spirals having negative and positive chiralities differ significantly in energy [see Fig. 1], which gives rise to strong antisymmetric exchange parameters. Moreover, a large number of metastable magnetic configuration of the bilayers have been calculated including the ground state and low-energy excited states. Here, the strong antisymmetric exchange has resulted in very complex magnetic textures including spin spirals and skyrmions [see Fig. 2].

Discussion

The main goal of this initial phase of the project was to

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demonstrate the general feasibility of our proposed approach to magnetic thin films. The so far obtained results are consistent with experimental and theoretical investigations on similar systems confirming the approach. The strength of the antisymmetric exchange is surprising and further calculations are needed to enhance our understanding of its origin. In the future, we would like to improve the DFT calculations in order to refine the parameters of the generalized Heisenberg models. We also plan to investigate the associated energy landscapes in detail including the metastable states and the transition states, which would provide information on both the equilibrium and also the dynamic properties of transition-metal bilayers. Moreover, we would like to include external magnetic and electric fields in our calculations to probe the possibility of manipulating these systems, for instance, by creating and annihilating skyrmions in specific spots.

Figures

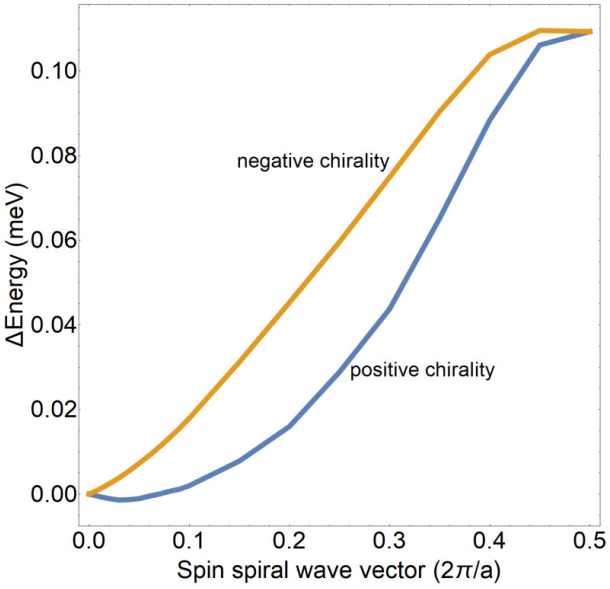


Figure 1: Frozen-magnon dispersion relations for positive (blue) and negative (orange) chiralities. From the differences between both curves, the antisymmetric exchange parameters can be obtained.

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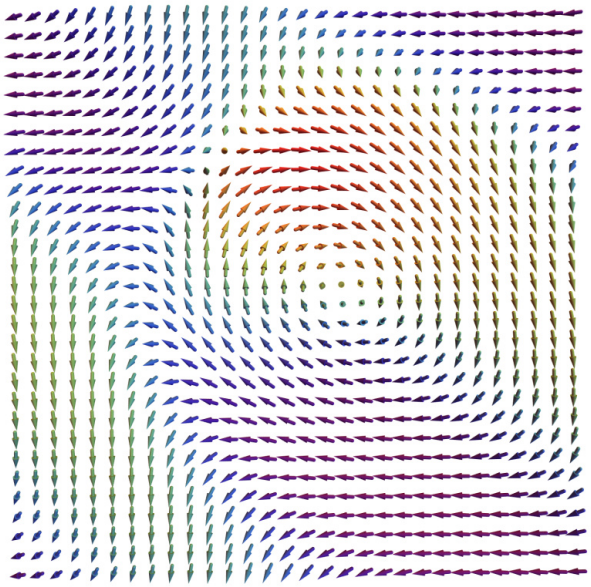


Figure 2: A metastable configuration containing a skyrmion obtained from the generalized Heisenberg model extracted from the frozen-magnon dispersion relations in Fig. 1. The colors of the arrows indicate the projection of the spins along the x direction.

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