

Search for next generation magnetic memory

First-principles study of topological spin textures at surfaces

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In Short

- Magnetic skyrmions are stable spin structures on the nanometer length scale with unique topological and transport properties which are promising for future magnetic memories.
- Using a multiscale approach combining electronic structure theory with Monte-Carlo and spin dynamics simulations we explore the properties of magnetic skyrmions at transition-metal interfaces.
- We strive at designing novel interfaces in order to tailor the properties of skyrmions such as their diameter, stability, critical fields and temperatures.

The magnetic phase space of nanostructures at surfaces and interfaces – potentially suited for applications in spintronics or data storage – is tremendously enhanced due to the interplay of a number of competing interactions. In particular, the Dzyaloshinskii-Moriya (DM) interaction can play a key role for ultra-thin films, clusters, or atomic chains at transition-metal surfaces. The DM interaction originates from spin-orbit coupling and can occur in every system with broken inversion symmetry such as surfaces and interfaces. Surprisingly, it had not been taken into account in such systems until in 2007 Matthias Bode and co-workers discovered that it can induce non-collinear spin structures in ultra-thin transition-metal films on surfaces [1]. Since then it has been found to be essential in many ultra-thin transition-metal films on surfaces and interfaces and can induce intriguing spin structures such as chiral domain walls and magnetic skyrmions.

The microscopic mechanism of the DM interaction in metals has been discussed by Fert and Levy [2]. The interaction between the magnetic moments of two atoms is mediated by conduction electrons which are subject to spin-orbit scattering at a third atom. Therefore, the strength of the DM interaction in such systems depends on the spin-orbit constant of the third atom which should be a heavy transition-metal e.g. W, Ir, or Pt in order to obtain large effects. The DM interaction can be calculated from first-principles based on density functional theory

(DFT)[3]. DFT calculations of the DM interaction using the FLEUR code [4] give a good agreement of the calculated periods of spin spirals with the experimental values [5].

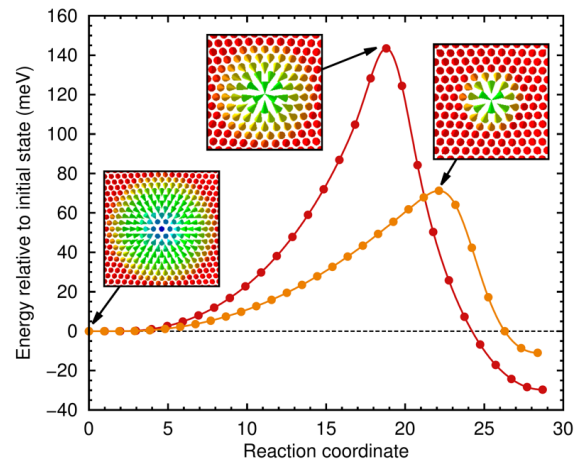


Figure 1: Energy barriers for the collapse of metastable skyrmions – tiny magnetic vortices with a diameter of just a few nanometres (see inset on the left) – into the ferromagnetic state (on the right of the reaction coordinate axis) via a transition state (see insets in the middle and on the right). The red curve shows a simulation based on parameters obtained from density functional theory while the orange curve is based on effective model parameters. The insets show the "atomic bar magnets" of each magnetic atom by a small coloured arrow. The red, upward-pointing arrows show a homogeneous ferromagnetic background. In the skyrmions the "atomic bar magnets" of the atoms spin around (orange and green arrows) and have an opposite orientation in their centres (blue arrows).

Even more spectacular is the recent discovery of magnetic skyrmions in ultra-thin transition-metal films at surfaces [7], [8]. Skyrmions are localized and topologically stabilized spin structures which occur in certain magnetic materials and which can be moved at current densities five orders of magnitude lower than those required for domain wall motion [6]. The spin structure of a skyrmion is shown in the right inset of Fig. 1. A key ingredient to stabilize skyrmions is the DM interaction as it induces a unique rotational sense of the spins from the core spins (blue arrows in the right inset of Fig. 1) to the ferromagnetic background (red arrows in the right inset of Fig. 1). In transition-metal ultra-thin films and interfaces, the interplay of exchange interaction, magnetocrystalline anisotropy, and DM interaction enhances the magnetic phase space tremendously. It cannot only lead to skyrmion lattice ground states such as discovered in an Fe monolayer on Ir(111) [7] but also isolated skyrmions can occur as recently observed in a Pd/Fe bilayer on Ir(111) [8] and ex-

plained based on first-principles calculations [9].

Skyrmions are also unfolding new physical phenomena such as the recently discovered *tunneling non-collinear magnetoresistance (NCMR)* [10]. In a tunnel junction with a nonmagnetic electrode the conductance changes in a skyrmion due to spin mixing resulting from its non-collinear spin structure. This discovery may facilitate the detection of skyrmionic bits in future spintronic devices.

In this project, we explore how the electronic and magnetic properties of interfaces can be manipulated e.g. by growing atomic overlayers of transition-metals, by alloying the substrate or by strain engineering in order to allow the occurrence of topologically non-trivial spin structures such as skyrmions or antiskyrmions [11]. Another type of systems considered here are magnetic multilayers that are better suited for transport measurements and manipulation at lower magnetic fields. In particular, we would like to find out in how far the properties of the skyrmions such as their diameter can be varied by the interface composition and to find systems that are suitable for transport measurements. Based on theory we have designed multilayer systems such that they can host skyrmions [12].

A key issue for applications is the stability of isolated skyrmions. We have shown that the energy barriers for collapse of individual skyrmions into the ferromagnetic state (see Fig. 1) and thus their lifetimes are greatly enhanced by frustration of exchange interactions [13] which are typical for itinerant electron magnets. In order to find systems in which skyrmions can be stabilized up to room temperature we study the phase diagram spanned by magnetic field and temperature of interface systems. So far, skyrmions have been found in ferromagnetic materials. Skyrmions in antiferromagnets have been predicted to show improved transport properties, however, to date they have not been observed experimentally. We study antiferromagnetic interfaces with large Dzyaloshinskii-Moriya interaction in order to identify promising systems [14].

We explore these issues based on a multiscale approach by combining density functional theory with Monte-Carlo and spin dynamics simulations. Both the ultra-thin films at surfaces as well as the multilayers are also studied by our experimental collaborators within the MAGicSky project.

WWW

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

More Information

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