Exchange interactions at the single atom and molecule level

Exchange interaction between a magnetic tip and single atoms or molecules on surfaces

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In Short

- Scanning probe microscopy (SPM) allows to measure the exchange forces between a magnetic tip and a magnetic surface on the atomic scale.
- Using density functional theory (DFT) the exchange interaction between a SPM tip and single atoms or molecules on surfaces is calculated.
- The direct observation of switching the magnetization of a single atom or molecule by exchange interactions in a SPM experiment is proposed.

Scanning probe microscopy plays a key role in nanoscience allowing to measure structural, electronic, magnetic, and chemical properties of atomic or molecular scale structures on surfaces. Nanostructures can even be built atom-by-atom by using the interaction with the tip of a scanning probe microscope. The development of spin-polarized scanning tunnelling microscopy (STM) [1,2] has opened the route towards exploring also magnetic properties on the atomic scale. Recently, it has become experimentally feasible to measure not only the spin-polarized current but also the exchange forces between a magnetic scanning probe tip and a magnetic nanostructure, a technique which has been coined magnetic exchange force microscopy (MExFM) [3,4].

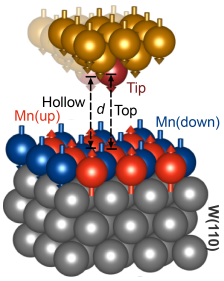

***Figure 1:** Perspective view of the Fe cluster SPM tip approaching the Mn monolayer on W(110) for an antiparallel alignment of the magnetic moments of the apex tip atom and the Mn surface atom underneath. Figure adapted from Ref. [5].*

In this project, we explore the interaction between magnetic tips and single atoms and molecules adsorbed on surfaces using DFT. One goal is to obtain the distance dependence of the exchange forces which can be directly compared to experiments performed by our collaboration partners. So far such force-distance curves have only been reported on ultrathin magnetic films [6] or on non-magnetic molecules [7]. We are collaborating with the group of Prof. Alexander Khajetoorians, University of Nijmegen, Netherlands on this project. His group has recently pioneered the development of a novel experimental technique combining spin-polarized STM with MExFM (coined SPEX), which allows probing simultaneously spin-polarized currents and exchange forces on the atomic scale.

As a model system for a complex noncollinear spin structure we have recently revisited a single atomic layer of Mn on the (110) surface of W, i.e. Mn/W(110) [5]. It has been previously shown that Mn/W(110) exhibits a cycloidal spin spiral with an angle of 173° between the magnetic moments of adjacent Mn rows due to the Dzyaloshinskii-Moriya interaction [8]. The group of Alexander Khajetoorians has recently been able to resolve the noncollinear magnetic order of Mn/W(110) with atomic resolution utilizing SPEX technique. Using distance-dependence spectroscopy, they quantified the exchange force and spin-polarized current on the top and hollow sites of the magnetic unit cell and found a strong variation in the exchange force signal [5]. Based on our DFT calculations, in which we considered both different surface positions and various tip terminations (see Fig. 1), we could explain these observations and how these measurements correspond to the spin-polarized currents obtained in parallel [5]. Using spin-resolved charge density difference plots, we demonstrate that the measured variation of the exchange forces are due to a competition of a short-range antiferromagnetic direct and a Zener-type long-range indirect ferromagnetic exchange mechanism which are particularly strong for Mn terminated tips (see Fig. 2).

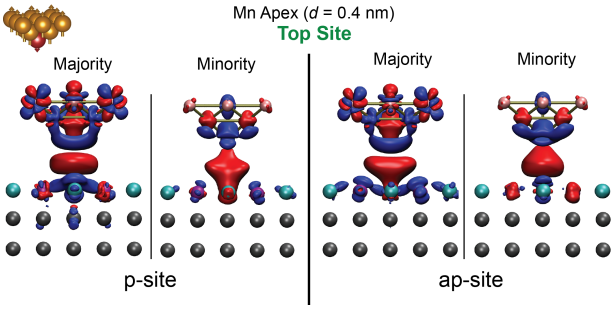

***Figure 2:** Spin-resolved charge-density difference plots along the [1$\bar{1}$0] direction for the interaction of Mn- and Fe-terminated tips with the Mn monolayer on W(110) at a tip-sample separation of d = 0.4 nm. Figure adapted from Ref. [5].*

In another recent work [9] we have demonstrated that an individual adatom on a magnetic surface can exhibit a noncollinear spin density. Using DFT we studied Co and Ir adatoms on Mn/W(110). Due to hybridization with the nearest and next-nearest Mn atoms of the monolayer the spin direction of the underlying substrate is encoded into the orbitals of the adatom. This explains recent scanning tunneling microscopy experiments showing a spin sensitive shape asymmetry of adatoms [10] which confirms the intra-atomic noncollinear magnetism of the adatoms.

We have also recently showed that Pb and Bi adatoms and dimers with their $6p$ electrons have large tunneling anisotropic magneto resistance (TAMR) when adsorbed on a magnetic surface due to strong spin-orbit coupling and the hybridization of molecular π orbitals with the magnetic surface [11]. Using DFT, we have explored the TAMR effect of $6p$ adatoms and dimers adsorbed on Mn/W(110). We have also investigated and compare structural and electronic properties of $3d$ transition metal adatoms on Mn/W(110) [12]. Due to the cycloidal spin spiral ground state, this surface acts as an excellent choice to explore the angular dependence of TAMR of adsorbed adatoms and dimers using scanning tunneling microscopy (STM). Investigating the anisotropy of the local density of states (LDOS) in the vacuum, we show small induced moments, however, large spin polarization and large TAMR for both adatoms and for suitably oriented dimers, which can be measured in STM experiment.

Another ongoing objective of this project is to demonstrate switching of the magnetic moment of a single atom by exchange interaction with a tip. Such a switching event can be experimentally verified by measurements of the tunnelling current. As the tip is approached towards the adatom, the exchange interaction between the magnetic moment of the tip apex atom and the adatom will drastically increase. From previous work on the exchange interaction between a magnetic tip and the surface atoms of an ultra-thin magnetic film it is known that the exchange energy can be on the order of 50-100 meV [6]. The magnetic moment of the adatom will be coupled to the magnetic substrate by exchange interaction on the order of a few ten meV.

There will be a competition between the exchange interaction between tip, adatom, and substrate. If the magnetic moment is in the alignment which is preferred by the exchange interaction with the tip, we do not expect a change upon approaching the tip. However, if the magnetic moment is in the opposite alignment due to the magnetization of the underlying substrate, we expect a flip of the moment of the molecule at close distance. Such a change of the magnetic moment direction will lead to a large change of the conductance due to the giant magnetoresistance [13,14]. Therefore, switching can be experimentally detected in a contact STM experiment performed for magnetic adatoms adsorbed on magnetic substrate. Within our project we would like to verify this proposal of switching the magnetic state and to identify promising systems for the experimental realization.

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

More Information

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