

## Exchange interactions at the single atom and molecule level

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

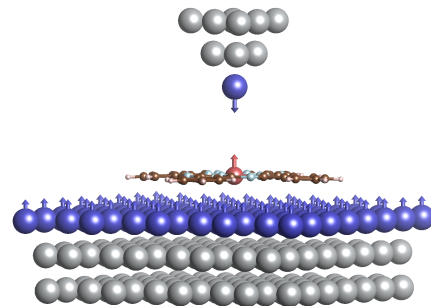
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#### In Short

- 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 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].

In this project, we explore the interaction between magnetic tips and single atoms and molecules adsorbed on surfaces using density functional theory. 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 [5] or on non-magnetic molecules (e.g. Ref. [6]). Another objective is to demonstrate switching of the magnetic moment of a single atom or molecule by exchange interaction with a tip. Such a switching event can be experimentally verified by measurements of the tunnelling current. The spin-polarized density functional theory calculations will comprise a large number of atoms due to the necessity of taking the tip explicitly into account and require to perform structural relaxations at every tip-sample distances. Therefore, they can only be carried out on supercomputers.



**Figure 1:** Sketch of the interaction between a magnetic SPM tip and a magnetic Pc molecule adsorbed on a magnetic surface. The exchange interaction between the magnetic moment of the tip apex atom (blue sphere) and the magnetic center of the molecule (red sphere) increases with decreasing tip-molecule separation and will compete with the exchange coupling of the magnetic molecule to the surface.

Fig. 1 shows a sketch of the interaction of a magnetic tip with a magnetic molecule adsorbed on a surface. As the tip is approached towards the molecule, the exchange interaction between the magnetic moment of the tip apex atom and the magnetic center of the molecule 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 [5]. The magnetic moment of the molecule 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 and molecule and between molecule 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 [7,8]. Therefore, switching can be experimentally detected in a contact STM experiment performed for magnetic molecules adsorbed on magnetic islands of opposite magnetization direction. Within our project we would like to verify this proposal of switching the magnetic state and to identify promising systems for the experimental realization.

### WWW

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

### More Information

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### Project Partners

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