Max Planck Institute of Microstructure Physics
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Magnetic Nanostructures

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An important focus of the group focus lies in the investigation of the electronic and magnetic properties of nanostructures at surfaces. Using state-of-the-art commercial and home-made density functional theory and kinetic Monte Carlo codes (software) we study, among other things, electronic properties of nanoscale surface structures, and spin dependent effects therein, to better understand how they can be controlled, measured, and possibly applied in modern technological challenges, such as the advancement of spin electronics (spintronics) and novel data storage development. And since for success of spintronics it is not sufficient to understand the intrinsic magnetic and electronic properties of nanostructures we also strive to find adequate means of controlling those properties externally. We study various possibilities for such external control, e.g. through applied electric field or the interaction with a scanning tunneling microscope tip. Another major focus of our research lies in self-organization. While modern experimental techniques allow one to assemble complex structures in an atom-by-atom fashion, this process is very cumbersome and cannot be applied in industrial applications. By understanding the interplay between electronic properties of nanosystems and their interaction we can force the nanostructures to self-assemble on a surface under certain environmental conditions. And finally, we endeavor to understand such properties of oxidic surfaces as their vibrational (phonon) spectra and their dependence on electronic and structural properties.

Spin dependent effects

To understand and control magnetism of surface nanostructures one has to understand and control the electrons at the surface. Numerous interesting effects can be observed and put to use at surfaces that contain the so-called Shockley surface state - a state localized near the surface and behaving as a quasi-2-dimensional electron gas. The electrons in this state scatter at surface impurities and if the impurities form a closed geometry, the surface

state electrons can become confined to that geometry. Carefully controlling the confinement shape one can deliberately channel and focus electrons. For example, it has been shown experimentally [1], that an elliptic atomic (quantum) corral can coherently transfer the information about the magnetic (Kondo) state of a single atom residing in one of its focal points to the other focal point. Using the Korringa-Kohn-Rostoker Green's function method we can fully ab initio calculate such complex multiple scattering problems (Fig. 1) [2].

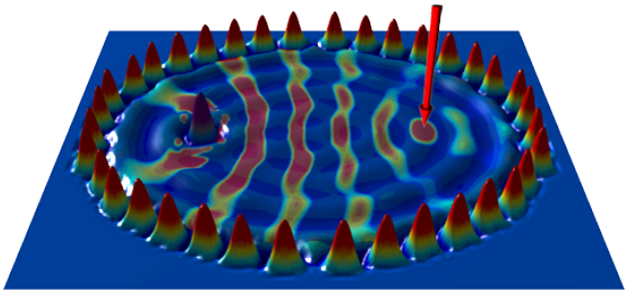

FIG. 1:

This amazing property of quantum corrals can be used to tailor magnetic interaction between single adatoms if those are placed in the focuses of the corral or even a part of a corral. Our calculations show that by carefully adjusting the size and shape of the corral one can enhance, quench or even reverse the coupling between individual spins at the surface (Fig.2) [2].

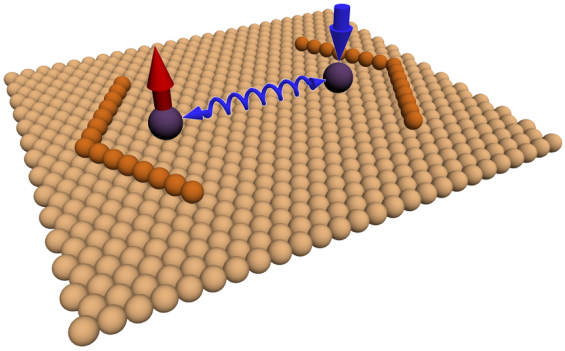

FIG. 2:

Yet it is not always necessary to use corrals, that are extremely hard to produce experimentally, to confine surface electrons. Natural or self-assembled surface structures can serve the same purpose. So, for example, our calculations have proven, that quantum confinement of surface state electrons on hexagonal copper islands can be used to tailor the interaction between single magnetic adatoms adsorbed on top of them (Fig. 3) [3].

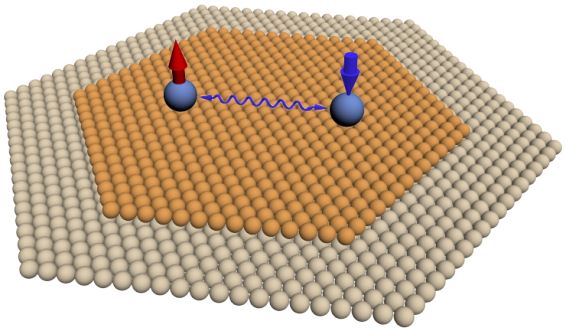

FIG. 3:

While confinement of surface state electrons by paramagnetic structures can aid in controlling the interaction of single magnetic impurities adsorbed within, the confinement itself can also be spin-dependent. So, e.g., our calculations have predicted that the spin-dependent confinement on triangular cobalt islands leads to a strong variation of the local magnetization within a single island/nanostructure [4]. Quite recently our predictions have been confirmed by our experimental colleagues (Fig. 4) [5].

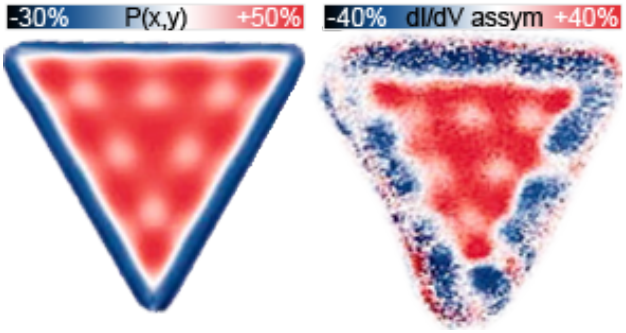

FIG. 4:

We also study other types of electron confinement. So, for example, electrons confined between a buried magnetic layer or cluster and the vacuum barrier at the surface of the crystal form quantum well states and can significantly affect the orientation of single spins at the surface (Fig. 5) [6].

Spin manipulation

While it is paramount to understand the intrinsic magnetic and electronic properties of nanostructures to learn to control them, it is equally important to find means of externally affecting those properties to ultimately gain control over magnetism gown to the single spin

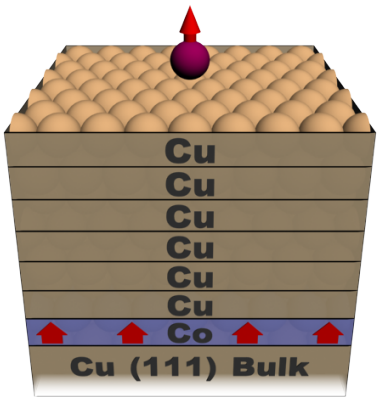

FIG. 5:

level. We thus strive to find such means. A powerful and, even more importantly, local way to affect the magnetic coupling in surface nanostructures is by using the electric field. Contrary to its magnetic counterpart, electric field can be delivered locally by means of a scanning tunneling microscope tip of a nanojunction. Our calculations show that external electric fields can control magnetism in bi- or even multi-stable magnetic units on a metal surface (Fig. 6) [7].

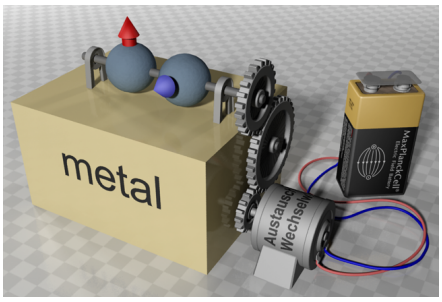

FIG. 6:

Another way of locally controlling the orientation of single spins is the use of a magnetic tip of a scanning tunneling (STM) or atomic force (AFM) microscope. We show that the spin orientation of single atoms and dimers on the surface and the conductance through those structures can be controlled by vertical or lateral movements of a spin-polarized STM tip (Fig. 7) or a finite bias applied to the tip-structure-substrate nanojunction [8, 9].

Dynamics and selforganisation

An ultimately important aspect of surface science is the ability to construct nanoscale systems and control their dynamics. The former is a prerequisite to any fundamental ex-

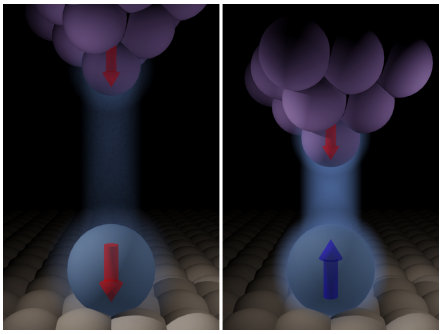

FIG. 7:

periment or industrial application and the latter is essential for assessment of the system's stability and evolution. We know that the dynamics of a system is intimately bound to the system's geometry and electronic structure. Understanding and controlling them means understanding and controlling the dynamics.

We use ab initio density functional theory methods to describe the underlying electronic effects and kinetic Monte Carlo simulations to reveal the dynamics of the system in real time. For example, precise description of the Shockley surface state [10] on a metal surface and its effect on the long ranged interaction of surface adsorbates allows us to accurately describe the dynamics of adatoms immersed in the 2D electron gas of the surface state. Our calculations predict that such dynamics may lead to the assembly of the adsorbates into a Kondo superlattice (Fig. 8 left) which lies in perfect agreement with experimental observations (Fig. 8 right) [11, 12].

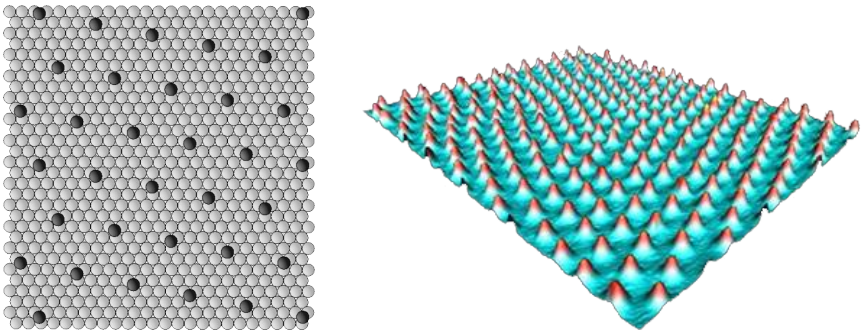

FIG. 8: Calculated (left) and experimental (right) Kondo superlattice.

On certain stepped surfaces the very same physics may lead, according to our calculations and experimental evidence of our colleagues [13], to the formation of one-dimensional nanostructures, i.e. atomic strings (Fig. 9).

Our calculations allow us to predict the dynamics of adatoms in more complex systems.

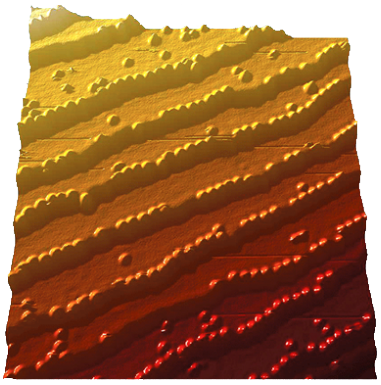

FIG. 9: Selfassembled atomic strings of [Fe/Cu(111)]

For example, in circular quantum corral, the diffusing adatoms would prefer to form concentric rings (Fig. 10), rearranging themselves in the semblance of a quantum onion [14]

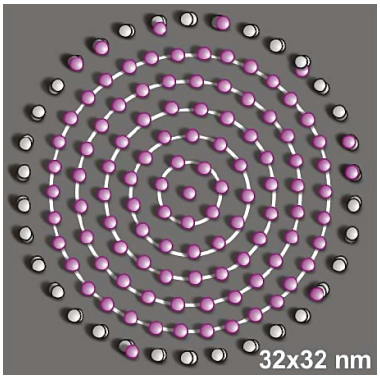

FIG. 10: Quantum onion

By careful choice of geometry one can use the electronic properties of the surface state to trap adatoms in otherwise open geometries. For example, the energy landscape for the diffusion of a single adatom formed by an open "quantum resonator" (Fig. 11) consisting of two parallel monatomic chains, causes the adatom adsorbed within to hop along linear channels and prevents it from leaving the resonator [15].

Oxidic interfaces

Our group also participates in the activities of the SonderForschungsBereich 762 of the German Science Foundation, in collaboration with experimental departments at our institute, as well as the Martin-Luther-Universität Halle-Wittenberg and universities of Leipzig and Magdeburg. Our main focus in the framework of SFB 762 is the study of elementary surface excitations, such as phonons and magnons, at oxidic surfaces. Using first principle

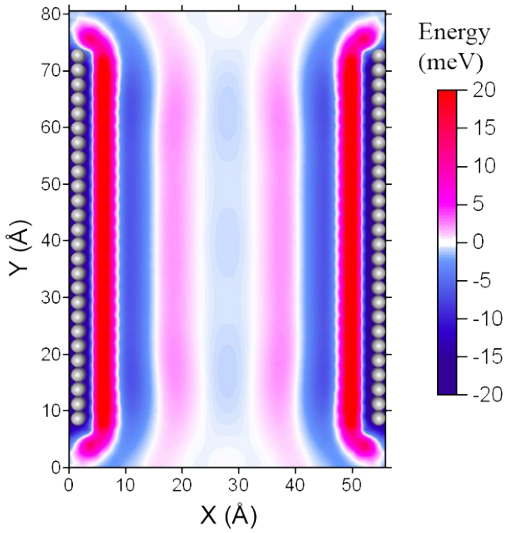

FIG. 11: Quantum resonator as a trap for diffusion adatoms

calculations we strive to avail our experimental colleagues from the experimental department I in understanding the exact nature of each experimentally observed excitation Fig. 12 [16].

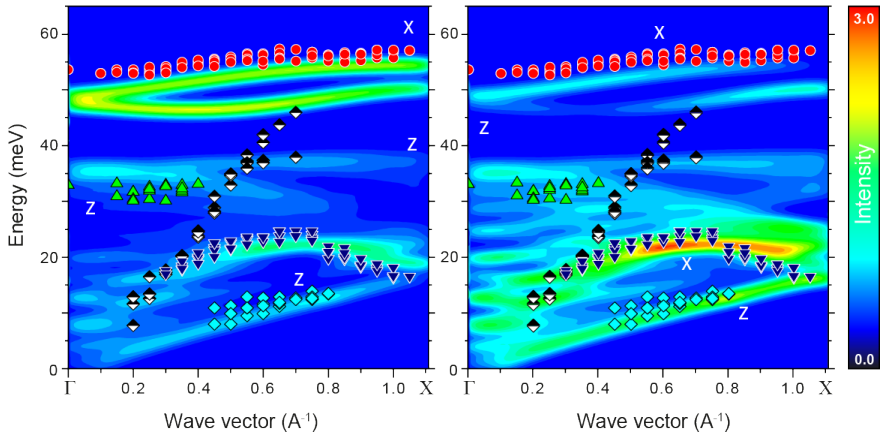

FIG. 12:

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