Scanning Tunneling Microscopy for Magnetic Molecules

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Magnetic molecules are among the most promising material systems for spintronics applications. Their small size together with the possibility of constructing large molecular superstructures make them an attractive platform for magnetic data storage. The understanding of their electronic structure and its correlation to their physical properties is a big challenge for both theory and experiment. From the theoretical point of view most of the existing *ab initio* approaches usually fail to describe properly the electronic structure of magnetic molecules as well as their physics. Furthermore the small size and reduced symmetry of molecules in general complicate the possibility of a detailed experimental characterization.

When deposited on surfaces at low coverage the sensitivity of the most commonly used experimental tools for investigating the electronic and geometric structure of materials are not sufficient. This problem can be overcome by using *Scanning Tunneling Microscope* (STM), which is a powerful technique for imaging surfaces at the atomic level. The high resolution provided by STM allows one to study of molecules and nanostructures on surfaces. STM can be also used to control and modify nanostructures [1], which makes it a suitable tool for investigating the physical properties of magnetic molecules.

The interpretation of the obtained STM images requires the modeling of the electronic structure. The most common theoretical scheme is based on the Tersoff-Hamann (TH) approximation [2], where the tip is assumed to be a single atom with s-like spherical symmetry. This model is widely used to relate the STM patterns and the electronic structure of systems under study. The general agreement between theory and experiment is mainly due to the recognition of certain symmetries that samples possesses. The TH model is however of limited use when the molecule has little symmetry and a simple *eyes-guided* comparison between theory and experiments is not informative. Furthermore neglecting the electronic structure of the tip may result is neglecting important features of the STM images, which are not attributable to the molecule to investigate but simply to the scanning tip.

We have developed a new computational scheme where both the tip and sample are treated on the same footing, and we were able the show that the geometry of the tip as well as its nature can dramatically change the simulated STM pattern. We did apply the model to Co-salen molecules on Cu surfaces and the agreement of both the topographic as well as the $\frac{dI}{dV}$ mapping with experiments is extremely good. We used for the basic electronic structure the *siesta* code [4], which employs local basis set and allows us to simulate such big molecules. The electronic structure obtained with *siesta* will be the input for simulating the STM images. As a benchmark we also plan to carry out transport calculations for the same molecules by using the non-equilibrium Green's function formalism as implemented in the *SMEAGOL* code[5] developed by our group. The STM of other molecules are simulated and compared to experiments.

References

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