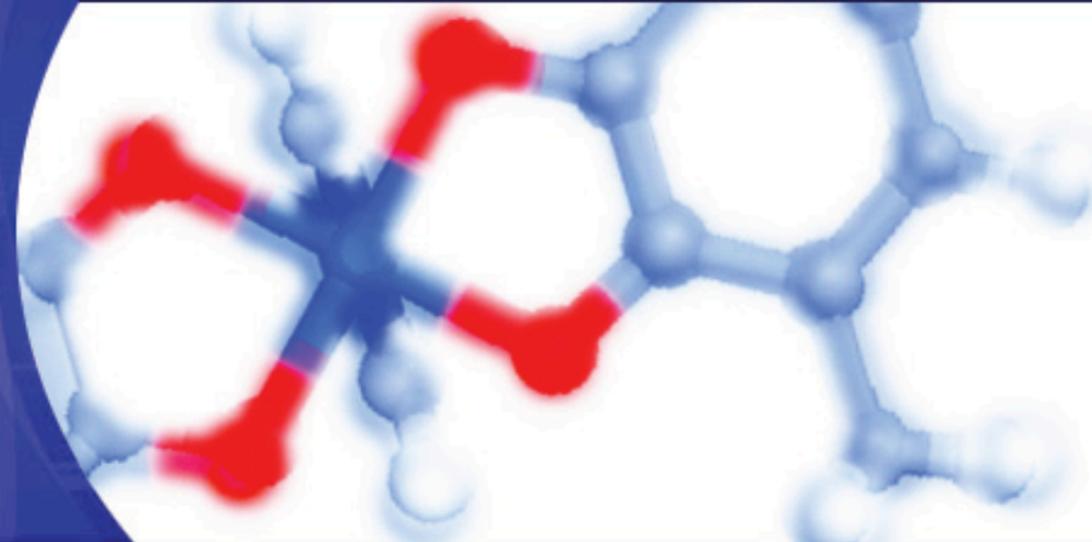


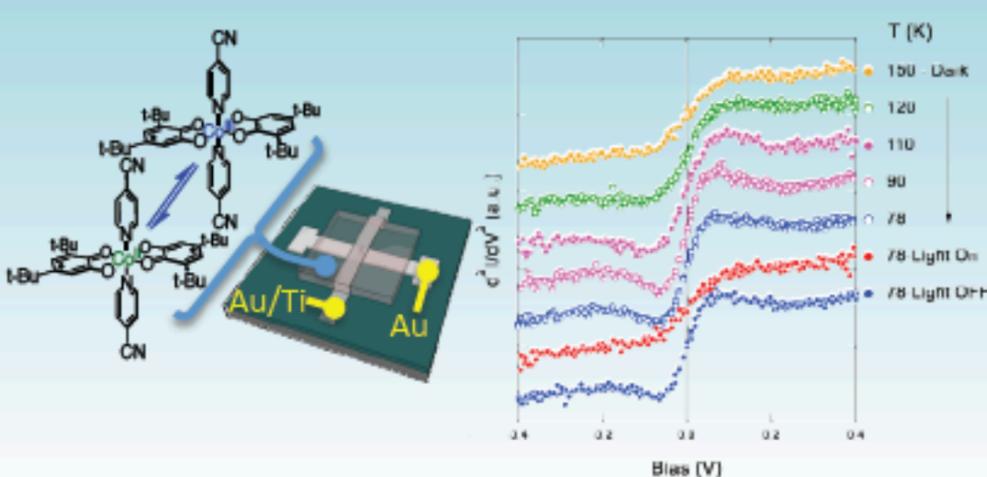
CENTER FOR MOLECULAR SPINTRONICS

2011 Year-end Report



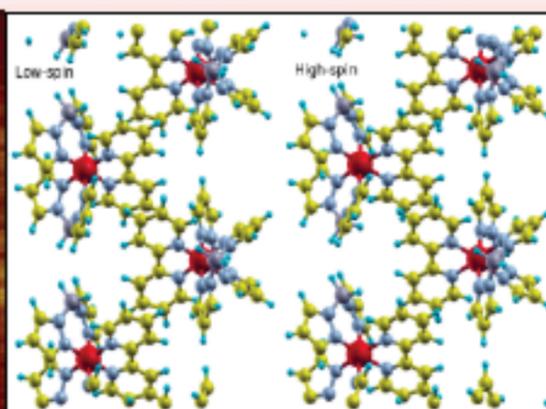
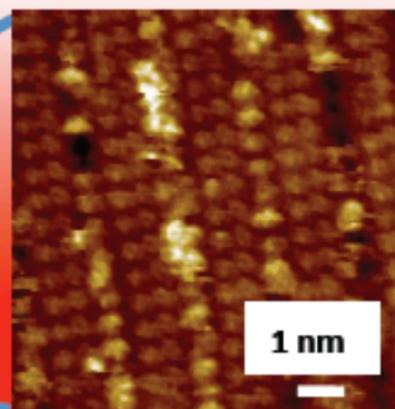
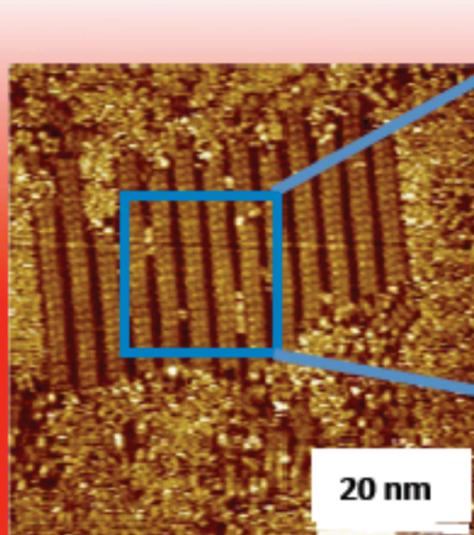
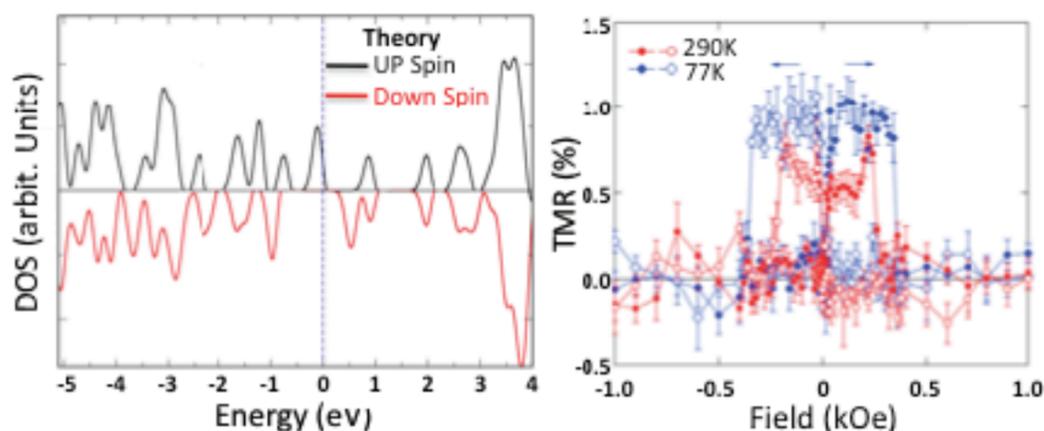
With the goal of driving development of new, energy-efficient spin-based molecular electronics, the Center for Molecular Spintronics studies the Chemical principles underlying current flow in such devices.

Greetings! In 2011, the Center for **Molecular Spintronics** made several exciting discoveries. The events and progress over the past 12 months include summer researchers from Shaw University, team-teaching our cross-listed Introduction to Magnetism and Magnetic Materials course and the observation of and theoretical support for molecule-actuated current changes in rudimentary devices. In addition, our Phase II team was assembled and includes 12 new PIs at 11 universities/institutes. The Phase II proposal was submitted in late September with the help of NCSU's Proposal Development Team.



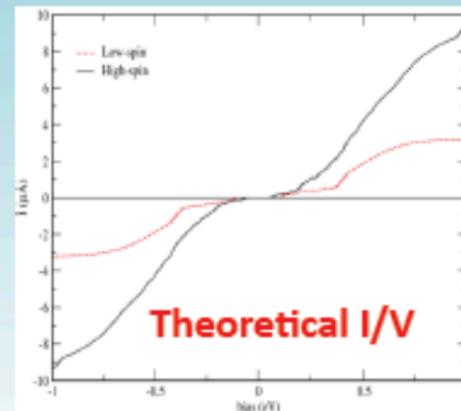
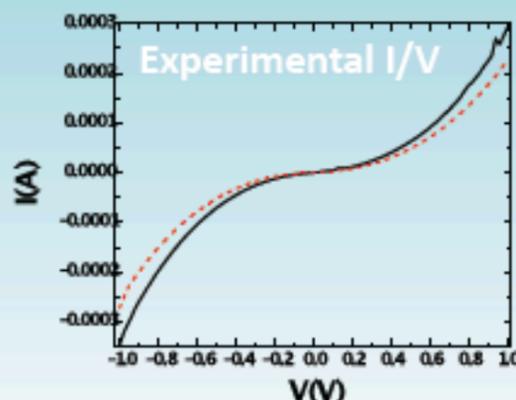
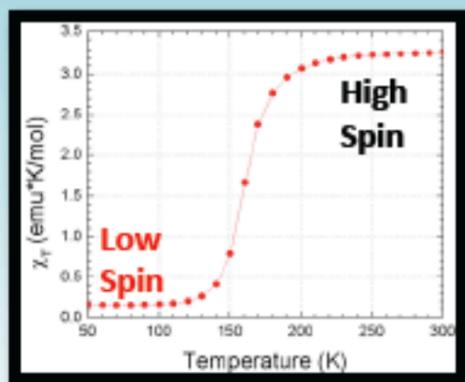
Will Rice (Tsui group/UNC Physics) and **Rob Bruce** (You group/UNC Chemistry) continue their work on switchable valence tautomer-based (**Dan Stasiw/Shultz** group, NCSU Chemistry) device. **Yifeng Chen** of the Buongiorno-Nardelli group (Physics, UNT) provided theoretical/computational support for differential conductivity for the two metastable forms of the valence tautomer. The resonances are peaks/dips in d^2I/dV^2 (\uparrow) and are switched-off by light (red curve), thus returning to the high temperature behavior (orange curve at 150K), illustrating that valence tautomers form the basis for a new type of molecular photoswitch device.

In addition, the theoretical density of states plot confirms the difference in minority and majority spin density conducive to the measured spin-valve effect (spin valve effect in permalloy/VT molecule/Co trilayer structure; $TMR = (R_{AP} - R_P) / R_P$) at two temperatures.



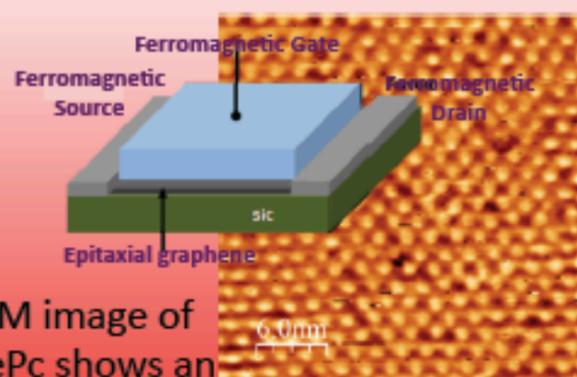
Alex Pronschinske (Dougherty group/NCSU Physics) is studying an Fe^{II} spin-crossover complex prepared by **Geoff Lewis** (Shultz Group).

Evaporated films on gold substrates show dimeric ordering similar to the molecular packing in the crystal...

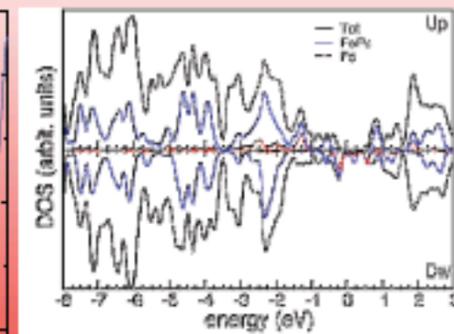
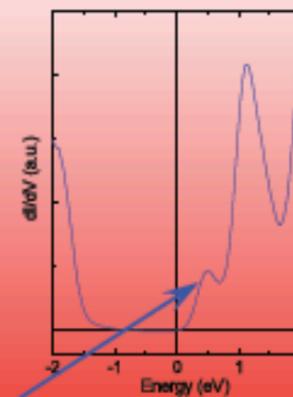
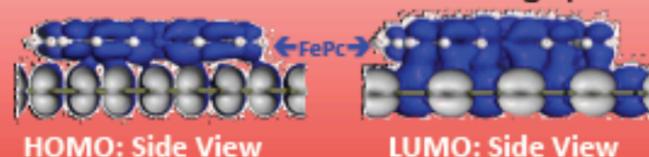


Experimental and theoretical current/potential (I/V) curves change as a function of temperature commensurate with the high-spin/low-spin change measured by SQUID magnetometry.

Andreas Sandin in the Rowe group (NCSU Physics) has found that iron phthalocyanine (FePc) molecules are more stable on graphene than on graphite. Experiment and Theory both show a strong molecule-graphene orbital mixing.

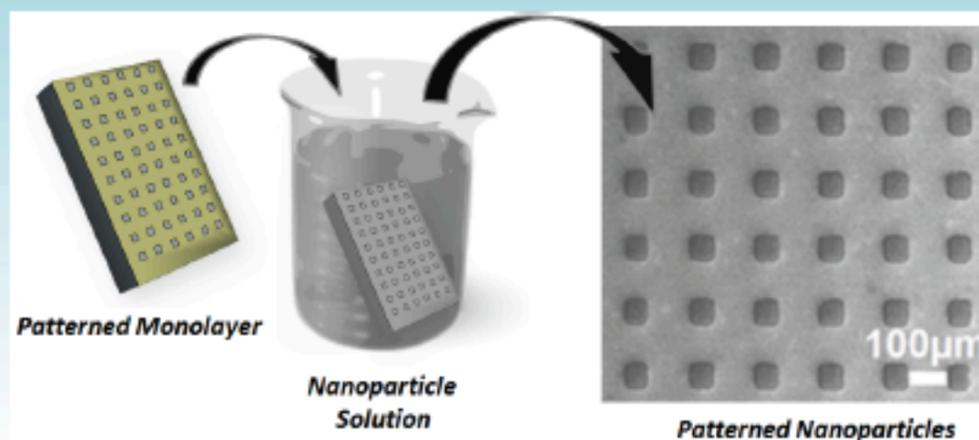


DFT calculations of the graphene/FePc interface show orbital mixing that explains structure and electronic tunneling spectra.

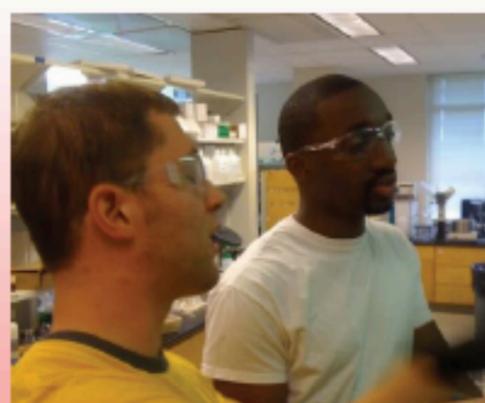


Experimental tunneling spectrum shows a mixed-orbital state near +0.5 eV, confirmed by theoretical DOS.

Yanni Jie (You group /UNC Chemistry) devised a method for laterally patterning Co, FePt, Fe₃O₄, Ni, and Au nanoparticles synthesized by **Aaron Johnston-Peck** and **Peter Krommenhoek** (Tracy group/NCSU Mater. Sci. & Eng.). Such patterned arrays will be used in future *Center* research projects.



As part of our Broadening Participation plan, the Center hosted three students from Shaw University. Partial funding for the students was provided by NCSU's RISF program and the Kenan Institute.



The students presented their work at the Center-wide poster session in August. PIs, students, postdocs and visiting faculty from several departments and universities attended.

Jones (NCSU Math, Science and Technology Education) and High School teacher/*Center* Kenan Fellow Liz Wollard led several teacher workshops.

