Magnetism and Lateral Ordering Phenomena of Switchable Molecules on Surfaces
or: What B3 of SFB 658 is doing

Lorenz Drescher

May 30th 2013
Outline

Methods of measurement
- XPS
- XAS
  - NEXAFS
  - XMCD

Studied Systems and Molecules
- Conformational Switches
- Spin-Crossover Switches
- Chemical Switching of Magnetic Properties

Outlook
- Magnetic Properties of Adsorbed Metal Complexes
- Molecular Switches on Magnetic Surface-Structures
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X-Ray Photoelectron Spectroscopy (XPS)

- Excitation of core-level electron over ionization barrier

from M. Bernien, X-Ray Absorption Spectroscopy of FE Complexes on Surfaces: Electronic Interactions and Tailoring of the Magnetic Coupling, FU-Berlin Diss. (2009)
X-Ray Photoelectron Spectroscopy (XPS)

- Binding energy depends on charge density
  - Chemical Shift

from Henzler & Göpel: Oberflächenphysik des Festkörpers, Teubner (1994)
X-Ray Absorption Spectroscopy (XAS)

- Excitation of core-level electron in unoccupied state close to the ionization barrier
- Density of empty states
  - Spin-state, oxidation, ligand-field
- Requires tunable X-ray source
  - Synchrotron

from M. Bernien, FU-Berlin Diss. (2009)

based on M. Bernien, Promotionsvortrag (2009)
Near Edge X-Ray Absorption Fine-Structure (NEXAFS)

- Element specific
- Probes unoccupied molecular orbitals
  - Chemical information
  - Orientation of orbitals
- Theoretical model via DFT

based on M. Bernien, X-Ray Absorption Spectroscopy of Fe Complexes on Surfaces: Electronic Interactions and Tailoring of the Magnetic Coupling, FU-Berlin Diss. (2009)
X-Ray Magnetic Circular Dichroism (XMCD)

- Element specific magnetic moments and magnetization

from M. Bernien, Promotionsvortrag (2009)
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Conformational and Ring-Opening/-Closing Switches

- Spiropyran ring opening
- Orientation of adsorbed molecules via NEXAFS
- Inhibiting interaction with surface

N 1s-XPS spectra of Spiropyran/Au(111) during heating. Both fig. from M. Piantek, FU-Berlin Diss (2009)
Conformational and Ring-Opening/-Closing Switches

- Spiropyran ring opening
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N 1s-XPS spectra of Spiropyran/Au(111) during heating. Both fig. from M. Piantek, FU-Berlin Diss (2009)
Adsorbed Spin-Crossover Switches

- Two metastable spin-states (low-spin and high-spin).
- Switchable by temperature, light, ...

Spin Crossover

\[ d^6 \]

low spin \quad \leftrightarrow \quad high spin

from M. Bernien: Spin Crossover in a Vacuum-Deposited Submonolayer of a Molecular Iron(II) Complex, DPG-Talk 2013

- Other talk
Reversible Switching of Magnetic Properties by Ad- & Desorption of NO.

- Planar molecules (metalo-porphyrins) allow for manipulation of metallic ion
- Adsorption of NO-molecule switches magnetic properties
- Reversible by desorption

from M. Bernien, FU-Berlin Diss. (2009)

from W. Kuch, et al., “Magnetismus und laterale Ordnungsphänomene von schaltbaren Molekülen auf Oberflächen”, Poster
Reversible Switching of Magnetic Properties by Ad- & Desorption of NO.


CoOEP on O-Ni/Cu(001) measured with p-linear polarized light at an angle of 20° at 130K. Desorption was ensured by heating to 350K. Spectra are shifted vertically. From C.F. Hermanns, et al., J. Phys.: Condens. Matter 24 394008 (2012)
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Outlook: Magnetic Properties of Adsorbed Metal Complexes

- Study influence of substrates to spin-cross-over switches
- Coupling surface - substrate of porphyrine & phtalocyanine
- Dual-core metal-complexes
  - Intramolecular coupling
  - Possible switching?

from W. Kuch, et al., “Magnetismus und laterale Ordnungsphänomene von schaltbaren Molekülen auf Oberflächen”, Poster
Outlook: Molecular Switches on Magnetic Surface-Structures

- De-couple switches from substrate
- Influences to magnetic properties of substrates
- Self-assembled networks
  - lateral coupling of molecules

from W. Kuch, et al., “Magnetismus und laterale Ordnungsphänomene von schaltbaren Molekülen auf Oberflächen”, Poster
Questions?