Low dimensional systems

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We study objects like **zero dimensional endofullerenes** and **two dimensional (2D) boron nitride** in view of their functionality as nano-materials.

Single molecule magnetism is the focus in the fullerene research, where we apply bulk sensitive x-ray absorption and a sub-Kelvin superconducting quantum interference device to the materials that we obtain from collaborations with synthesis groups.

In the 2D activity we aim to **grow highest quality boron nitride** on substrates with chemical vapour deposition methods and subsequent **exfoliation** of single layers. For this purposes we use a clean room, optical microscopy, transmission electron microscopy and surface science methods such as low energy electron diffraction, photoemission and scanning tunneling microscopy.

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Electrostatic Interaction across a Single-Layer Carbon

Low dimensional systems like single layer boron nitride or fullerenes, both realise membranes that separate two regions. Though these ultimately thin single layer membranes allow chemical interaction across the membrane. For example, electrons may easily tunnel across single layer boron nitride, or the carbon cage of a fullerene molecule does not realize a Faraday cage that completely shields the electrostatic field of the endohedral unit [1]. This is reminiscent to proximity effects as observed in magnetic interfaces or in superconductors. It is a manifestation of physics at the nanometer scale and may possibly be exploited in future nanodevices. In the case of magnetic endofullerenes electrostatic control will open new possibilities of addressing the spin information inside the molecules.

Specifically, we investigated the single molecule magnet $\text{TbSc}_2\text{N}@\text{C}_{80}$ [1]. Over all, the molecule is neutral and has a very small dipole moment. The TbSc_2N endohedral unit transfers six electrons on the carbon cage. The resulting



Electrostatic potential of a C_{80} endohedral fullerene. (a) Calculation of the potential of $YSc_2N@C_{80}$ on a plane comprising the endohedral cluster and the carbon shell (contour units meV). (b) High resolution x-ray photoelectron spectroscopy from the carbon shell of $TbSc_2N@C_{80}$ (red dots) and comparison to the calculated C1s eigenvalues that mainly reflect the electrostatic potential at the 80 carbon sites (grey bars and black line) (from [1]).

discrete charge distribution causes an electrostatic potential that is not spherical and thus not constant outside the molecule. The figure above shows the calculated electrostatic potential. As expected, it falls off rapidly but has a significant non-isotropic component outside the carbon cage. The potential in the immediate vicinity of the cage may not be measured easily, though it can be inferred from the potential at the positions of the carbon atoms. The potential variation on the carbon cage is reflected in the electron binding energies as they are measured with photoemission. We could establish the correlation between the calculated C1s eigenvalues and the measured C1s core level binding energies. Due to the high requirements to the energy resolution the experiments were performed at the photoemission and atomic resolution laboratory (PEARL) beamline at the Swiss Light Source.

Highlighted Publications:

1. Electrostatic interaction across a single-layer carbon shell

R. Stania et al., J. Phys. Chem. Lett. 9 3586 (2018)

2. Remote doping of graphene on SiO_2 with 5 keV x-rays in air

B. Salzmann *et al.*, J. Vac. Sci. Technol. A **36** 020603 (2018)

- Centimeter-sized single-orientation monolayer hexagonal boron nitride with or without nanovoids H. Cun *et al.*, Nano Letters **18** 1205 (2018)
- Orbital insight from an upright molecule T. Greber, Nature 558 525 (2018)