Low dimensional systems

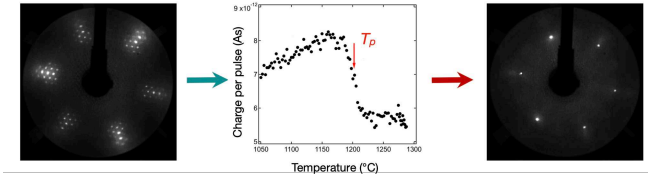
Prof. Thomas Greber

We study objects like **zero-dimensional endofullerene** molecules and **two-dimensional (2D) boron nitride** layers in view of their functionality as nano-materials. Single-molecule magnetism is the focus of the fullerene research, where we apply x-ray absorption and a sub-Kelvin superconducting quantum interference device. In the activity of the 2D materials, we grow the highest quality boron nitride on substrates up to the four-inch wafer scale with chemical vapor deposition, subsequent exfoliation, and implementation in devices. At UZH Irchel, we use a dedicated clean room, optical microscopy, inkjet printing, and surface science tools such as low-energy electron diffraction, photoemission, and scanning tunneling microscopy for these purposes. At the Swiss Light Source, we perform photoemission and x-ray absorption spectroscopy experiments.
https://www.physik.uzh.ch/g/greber

Stability of single layer *h*-BN on metals

High quality single layer hexagonal boron nitride may be grown on transition metals with chemical vapor deposition (CVD). These systems are used as templates for molecules, production of pores with nanometer size, functional electrodes in electrochemical cells, or as educts for the production of free standing boron nitride layers.

With density functional theory (DFT) we calculated the atomic adsorption energies of boron and nitrogen, BN dimers, $(BN)_3$ hexamers and *h*-BN with and without atomic vacancies for different transition metals. It turns out that the catalytic substrates lower the stability of the *h*-BN that is e.g. more stable on copper than on nickel. Importantly, defects, impurities like carbon or domain boundaries lower the stability of the systems. The over all stability may be quantified with pyrolysis experiments where the systems are heated at a given rate to high temperatures. The disintegration of the



Pyrolysis of h-BN on Pt(111). Low energy electron diffraction (LEED) pattern (E = 100 eV) prior (left) and after (right) pyrolysis. Center UV flash lamp photoemission signal during annealing with a heating rate of 10 °C min^{-1}. A significant signal drop is observed after the temperature reached the pyrolysis temperature T_p of 1200 °C (red arrow). Data: A. Hemmi et al., Small (2022).

h-BN is measured in the decrease of the photoelectron yield of a xenon flash lamp. For the case of *h*-BN on platinum the Figure shows high quality electron diffraction pattern of *h*-BN on Pt(111) before and clean Pt(111) after heating. The record pyrolysis temperature T_p of 1200 °C indicates highest quality boron nitride.

The pyrolysis temperature of *h*-BN on a given transition metal is a measure for its quality and can be correlated to the DFT results.

The calculations run at the at the Swiss National Supercomputing Centre (CSCS) in Lugano, and the experiments were performed in the Sinergia lab on the Irchel campus of the University of Zürich. The project was funded by the European Commission (European Union's Horizon 2020 research and innovation programme) under the Graphene Flagship.

Highlighted Publications:

1. Growing sp^2 materials on transition metals: calculated atomic adsorption energies of hydrogen, boron, carbon, nitrogen, and oxygen atoms, C_2 and BN dimers, C_6 and $(BN)_3$ hexamers, graphene and *h*-BN with and without atomic vacancies
   A. P. Seitsonen and T. Greber, Nanoscale Adv. **6**, 268 (2024)
2. Correlation of Work Function and Conformation of C_{80} Endofullerenes on *h*-BN/Ni(111)
   R. Stania *et al.*, Adv. Mater. Interfaces 2300935, (2023)
3. Inferring the Dy-N axis orientation in adsorbed $DySc_2N@C_{80}$ endofullerenes by linearly polarized x-ray absorption spectroscopy
   R. Sagehashi *et al.*, Phys. Rev. Mat. **7**, 086001 (2023)