From Magnetism to Catalysis: A Porphyrin-Based Multifunctional Interface

A. Windischbacher[1], H.M. Sturmeit[2], J.E. Nitschke[2], I. Cojocariu[3], V. Feyer[3], G. Zamborlini[2], P. Puschnig[1]

[1]*Institute of Physics, University of Graz, Austria*
[2]*Department of Physics, TU Dortmund University, Germany*
[3]*Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich, Germany*

Nature famously relies on porphyrin molecules for various processes such as photosynthesis or oxygen transport. It does so, as porphyrins can feature a variety of metal atoms and therefore offer great variability in stabilizing reactive or uncommon metal oxidation states. Transferring such metalloporphyrins onto surfaces extends their variability to the periodic regime, creating interfaces with appealing electronic and magnetic properties.

In this talk, I will introduce you to a biomimetic interface consisting of Nickel-tetraphenylporphyrin (NiTPP) and a Cu(100) surface. By combining various experimental methods with density functional theory simulations, we have investigated the on-surface electronic properties of NiTPP. In particular, we have studied the strong charge transfer from the surface to the molecule, which chemically activates the Ni ion. By analysing the different spin and oxidation states of the system, we further explain the consequences of the charge transfer for the interaction of NiTPP with small gases and its applicability in catalysis.