

Coordination-induced spin state switching of a new complex on surfaces

**Manuel Gruber^{a,b}, Alexander Köbke^b, Florian Gutzeit^c,
Rainer Herges^c, Richard Berndt^b**

^a*Faculty of Physics and CENIDE, University of Duisburg-Essen, Germany*

^b*Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Germany*

^c*Institut für Organische Chemie, Christian-Albrechts-Universität zu Kiel, Germany*

Switching the spin of metal-organic complexes on surfaces is attractive for its potential applications in, e.g., molecular spintronics. Intrinsic molecular switches such as spin-crossover complexes so far suffer from fragmentation or loss of functionality upon adsorption on metal surfaces [1] with rare exceptions [2]. Robust metal-organic platforms such as phthalocyanine- or porphyrin-based complexes, on the other hand, rely on external axial ligands to induce spin switching [3]. Yet, adding and removing axial ligands require particular conditions, which tend to affect the selectivity and reversibility of the switching process.

In the present study, we have designed and investigated robust Ni complexes, which can intrinsically switch their coordination state. The switching is based on a mechanical movement of an axial pyridine ligand strapped to a porphyrin. Using x-ray absorption spectroscopy and x-ray diffraction spectroscopy we evidence that the spin and coordination switching are interlocked. Furthermore, employing low-temperature scanning tunnelling microscopy, we show switching of individual Ni complexes in direct contact to a Ag(111) surface. The stability of the two spin and coordination states of the molecules exceeds days at 4 K [4].

This work was supported by the DFG through SFB 677 and the European Union's Horizon 2020 programme (No. 766726).

[1] Knaak *et al.*, *J. Phys. Chem. C* **123**, 4378 (2019).

[2] Bairagi *et al.*, *Nat. Commun.* **7**, 12212 (2016).

[3] Wäckerlin *et al.*, *Nat. Commun.* **1**, 61344 (2010).

[4] Köbke *et al.*, *Nat. Nanotechnol.* **15**, 18 (2020).