O 38: Invited Talk (Stefan Heinze)

Time: Wednesday 9:30–10:15 Location: TRE Phy

Invited Talk O 38.1 Wed 9:30 TRE Phy

Understanding STM experiments on single-atom junctions from first-principles — •Stefan Heinze — Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universtität zu Kiel, Germany

Today, scanning tunneling microscopy (STM) allows to create artificial nanostructures at surfaces atom-by-atom and to locally probe their structural, electronic, magnetic, and transport properties at the atomic level. In order to understand such experiments it is often indispensable to use a first-principles approach based on density functional theory. It is particularly intriguing to explore physical properties at the single atom limit. Here, I will show that it is possible to image the spin direction of single magnetic atoms on surfaces [1] and how the spin-valve effect in single-atom junctions can be explained [2]. We found that in such experiments the interaction between tip and adsorbed atom can become essential [3]. Surprisingly, it is also feasible to detect the spin-quantization axis of single atoms using non-magnetic STM tips [4] due to spin-orbit coupling. This effect – the so-called tunneling anisotropic magnetoresistance – can be implemented into a simple model of STM which allows fast simulation of spin-polarized and non-spin-polarized STM images [5].

[1] D. Serrate *et al.*, Nature Nanotech. **5**, 350 (2010).
[2] M. Ziegler *et al.*, New J. of Phys. **13**, 085011 (2011).
[3] C. Lazo *et al.*, Phys. Rev. B **86**, 180406 (R) (2012).
[4] N. Néel *et al.*, Phys. Rev. Lett. **110**, 037202 (2013).
[5] K. von Bergmann *et al.*, Phys. Rev. B **86**, 134422 (2012).