O 21: Invited Talk Hofer

Time: Tuesday 10:15–11:00 Location: H36

Invited Talk O 21.1 Tue 10:15 H36

Recent advances in simulating high-resolution scanning tunnelling microscopy and spectroscopy — •Werner Hofer — Liverpool Institute of Nanoscale Science, Engineering and Technology, Liverpool, UK

Since its invention scanning tunnelling microscopes have rapidly become the key instrument not only for the atomic scale analysis of surfaces, interfaces, and molecular structures, the instrument*s resolution has made it increasingly possible to detect electronic processes which before remained elusive. Driven by experimental advances sophisticated theoretical techniques have been developed, which make direct comparisons with quantitative results a close to routine procedure. The key ingredient in these techniques is the inclusion the STM tip in the simulations, and the use of highly accurate electronic structure methods. We provide several examples of the present state of theory, ranging from traditional problems of adsorption and catalysis[1], single adatom properties[2], to new magnetic structures, organic interfaces, and semiconductors[3]. Particular emphasis shall be placed on functionalising interfaces and molecular structures, which can be analyzed in great detail by STM[4-6].

[1] F Calleja et al. Phys. Rev. Lett. 92, 206101 (2004) [2] L. Limot et al. Phys. Rev. Lett. 94, 126102 (2005) [3] L. Zotti, W. A. Hofer and F. Giessibl, Chem. Phys. Lett. 420, 177 (2006) [4] P. Piva et al., Nature 435, 658 (2005) [5] S. Dobrin et al., Surf. Sci. Lett. 600, L43 (2006) [6] Z. T. Deng et al., Phys. Rev. Lett. 96, 156102 (2006)