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S e m i n a r

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DTU Building 311, meeting room, ground floor

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"Dynamic processes observed by scanning tunnelling microscopes: conformation changes, diffusion and vibrations"

Abstract:

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 of the STM tip in the simulations, and the use of highly accurate electronic structure methods. In this talk we shall focus on dynamic processes, which increasingly play an important role in state-of-the-art experiments. We shall limit our presentation to two fields of research: magnetic nanostructures and molecular corrals. In particular we show that the field-induced diffusion of adsorbates to the probe tip can change the magnetic resolution in the experiments by nearly one order of magnitude [1], and that the tip field will change the Kondo temperature of a single magnetic impurity in a continuous manner during its approach [2,3]. In case of single Ce adatoms on silver we find that a Kondo-like feature, which is only observed under particular experimental conditions, is due to hydrogen diffusion and subsequent vibrational excitations [4]. This is also important in the context of a previously reported Kondo effect for the Ce/Ag system [5], which in light of the theoretical analysis and new experimental evidence has to be subject to revision. Our second focus, molecular corrals on silicon surfaces, starts with an analysis of semiconductor properties upon adsorption of highly polar chlorododecane molecules [6,7]. Here, we show that the induced surface dipole due to the polar charge distribution changes the bandstructure of the semiconductor within the molecular corral to an extent usually observed only after semiconductor doping. Most interestingly, this effect is revealed as a consequence of only minor changes of the molecular conformation [8]. This research seems to open up the possibility of tailoring local semiconductor properties by molecular adsorption.

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[2] L. Limot et al. *Phys. Rev. Lett.* **94**, 126102 (2005)

[3] N. Neel et al. *Phys. Rev. Lett.* **98**, 016801 (2007)

[4] WA Hofer et al., *Nano letters*, submitted

[5] J. Li et al., *Phys. Rev. Lett.* **80**, 2893 (1998)

[6] S. Dobrin et al., *Nanotechnology* **18**, 044012 (2007)

[7] S. Dobrin et al., *Surf. Sci. Lett.* **600**, L43 (2006)

[8] KR Harikumar et al., *JACS* **128**, 16791 (2006)