

O 23 Invited talk Schmidt

Time: Tuesday 14:45–15:30

Room: TRE Phys

Invited Talk

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Organic molecule adsorption on solid surfaces: Chemical bonding, mutual polarisation and dispersion interaction*

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Many new and exciting electronic devices are based on the organic functionalisation of semiconductor surfaces. Weak interactions of molecules with template substrates, on the other hand, allow for studying molecular self-organisation at the fundamental level.

Here I discuss some of the most relevant bonding scenarios for the adsorption of organic molecules on solid surfaces from the perspective of first-principles calculations. Covalent bonds formed with semiconductor surfaces significantly modify the structural and electronic properties of both the adsorbed molecules and the substrate [1,2]. In many instances of organic molecule adsorption on metals, mutual polarisation leads to substantial charge transfer and re-hybridisation, despite small adsorption energies [3]. Subtle effects related to the lowering of the kinetic energy of the valence electrons as well as dispersion forces, finally, govern the interaction between the organic molecules and chemically inert substrates such as graphite [4].

*in collaboration with F. Bechstedt, F. Fuchs, K. Seino, M. Preuss (Jena) and A. Hermann (Auckland).

[1] K Seino, WG Schmidt, F Bechstedt, PRB 69, 245309 (2004).

[2] A Hermann, WG Schmidt, F Bechstedt, JPCB 109, 7928 (2005).

[3] M Preuss, WG Schmidt, F Bechstedt, PRL 94, 236102 (2005).

[4] F Ortman, WG Schmidt, F Bechstedt, PRL 95,186101 (2005).