Where catalysis meets molecular electronics:
Fundamental properties of physisorbed molecules.

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Although the importance of pyhsisorption and weak chemisorption for heterogeneous catalysis, the bonding of molecules to substrates and molecular electronics is not obvious there are quite a few situations where details of this interaction become important. It will be demonstrated that for phenomena like CH-bond activation of saturated hydrocarbons on metal surfaces [1,2] and charge-injection at the metal/organics interface [3] precise knowledge about the balance between the attractive dispersion forces and Pauli repulsion is required. Since these interactions cannot easily be accessed by the standard theoretical tool for analyzing adsorbate/surface interactions, density functional theory, or DFT, we will present results obtained by precise, wave-function based ab-initio methods, where dispersion forces are included on the level of second-order perturbation theory (MP2). Together these examples demonstrate that physisorption and weak chemisorption are not well-understood phenomena and call for more work, both experimental and theoretical.

[1] K.A. Fosser, R.G. Nuzzo, P.S. Bagus, Ch. Wöll,
Angew. Chemie **114**, 1811, (2002)

[2] K.A. Fosser, R.G. Nuzzo, P.S. Bagus, Ch. Wöll, J. Chem. Phys.
118, 5115 (2003)

[3] P.S. Bagus, V. Staemmler, Ch. Wöll, Phys. Rev. Lett. **89**, 096104 (2002)