

**PHYSICAL COLLOQUIUM**  
**INVITATION**

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Monday, 18.06.2018, 4.15 p.m., W2-1-148

speaks

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about

**Bonding behavior and magnetism of**  
**transition metal atoms on 2D materials**

Two-dimensional (2D) materials are of large interest for spintronics [1], in particular if transport can be influenced by accessory magnetic degrees of freedom [2].

In this talk I will discuss strategies how to couple magnetic atoms to 2D electronic systems. Hereby we are especially interested in minimum invasive methods such as deposition of magnetic atoms at low kinetic energies, which leaves the crystal structure of the host 2D system intact. At the same time, however, a minimum electronic and magnetic coupling of adatoms to the substrate is required in order to influence 2D transport.

I will present fundamental studies of chemical bonding and magnetic moments of 3d metal adatoms on inert 2D graphene and bismuth chalcogenide topological insulators. Experimental data with high surface sensitivity is acquired using x-ray magnetic circular dichroism (XMCD), photoemission spectroscopy (UPS, XPS), and scanning tunneling microscopy (STM) techniques.

In the case of graphene surfaces, magnetic adatoms tend to remain van der Waals bound, which represents the weakly coupled regime of localized quasi-free spins [3]. We show that in contrast to density functional theory (DFT) methods, quantum

chemistry calculations including long-range interactions can describe adsorption processes on realistic graphene systems well. The adatom's d-shell occupation and spin configuration depends on complex charge transfer effects at the graphene interface.

On the other hand for bismuth chalcogenide topological insulators Bi<sub>2</sub>Se<sub>3</sub> and Bi<sub>2</sub>Te<sub>3</sub> [4, 5] we observe a heavy relaxation of adatoms into the surface, despite the inert nature of these van der Waals stacked substrates. Here DFT methods can be applied, and we show that the hybridisation of d-states with the host band structure can even quench the adatom's moment entirely.

Our results show that the delicate interplay between long-range and local chemical bonding of adatoms on inert 2D surfaces makes resulting physical properties highly dependent on the material combination particular the choice of 3d metal element. The influence of van der Waals type long-range interactions, however, could be to a certain extent tuned by heterostructure concepts.

[1] S. Z. Butler et al., ACS Nano 7, 2898–2926 (2013)

[2] M. Piquemal-Banci et al., J. Phys. D: Appl. Phys. 50, 203002 (2017)

[3] V. Sessi et al., New Journal of Physics 16, 062001 (2014) [Fast Track Communication]

[4] J. Honolka et al., Phys. Rev. Lett. 108, 256811 (2012)

[5] M. Vondracek et al., Phys. Rev. B 94, 161114(R) (2016)

All interested persons are cordially invited.

Sgd. Prof. Dr. Martin Holthaus