



Department Seminar:

Monday, December 11, 2017, at 11:00 a.m.;

— all are invited to meet at around 10:40 for a chat and coffee —

Prof. Dr. Michael Rohlfing Elektronic Structure and Dynamics of
Condensed Matter,
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Electronic spectra of layered materials and monolayer adsorbates

PC Seminar Room G2.06, Building G, Faradayweg 4

J. Stähler

Abstract:

Many-body perturbation theory (MBPT) has emerged as a powerful tool for addressing electronic and optical spectra in low-dimensional systems. On the one hand, MBPT has sufficient predictive power to describe excited electronic states quantitatively. On the other hand, it allows to identify important properties and features of the electronic structure, like the role of spatial extent and overlap of quantum-mechanical states, or image-potential effects due to environment polarizability. Such features and mechanisms are shared by systems that appear quite diverse at first glance, like topological insulators and molecular adsorbates, but can nonetheless be addressed by the same computational approach. We will discuss some recent examples:

- (i) Topological insulators like Bi_2Se_3 exhibit metallic surface states (Dirac cone); in thin films these states hybridize and split [1];
- (ii) Exciton states in monolayers of transition-metal dichalcogenides are considered important for future optoelectronics; these states are significantly affected by geometrical deformation, doping, and substrate polarizability [2];
- (iii) Organic adsorbates on metal surfaces show characteristic molecular states which can even lead to Kondo resonances [3,4].

[1] T. Förster, P. Krüger, and M. Rohlfing, *Phys. Rev. B* **92**, 201404(R) (2015)..

[2] M. Drüppel, T. Deilmann, P. Krüger and M. Rohlfing, *Nat. Comm.* (2017).

[3] T. Esat, T. Deilmann, B. Lechtenberg, C. Wagner, P. Krüger, R. Temirov, F.B. Anders, M. Rohlfing, and F.S. Tautz, *Phys. Rev. B* **91**, 144415 (2015)..

[4] T. Esat, B. Lechtenberg, T. Deilmann, C. Wagner, P. Krüger, R. Temirov, M. Rohlfing, F.B. Anders, and F.S. Tautz, *Nature Physics* **12**, 867 (2016)..