3 years PostDoc position

at the Chair of Atomistic Modelling and Design of Materials, University of Leoben, Austria
http://www.unileoben.ac.at/amadm/

dedicated to

Electronic and Optical Properties of Organic Molecule / Metal Interfaces

We announce an opening for a PostDoc position in theoretical solid state physics with a focus on electronic structure calculations within DFT for the interface of organic molecules and metal surfaces. A major computational task of the project is the sub-monolayer to monolayer adsorption of functionalized organic molecules on various substrates. One important methodological development concerns the correct handling of van der Waals (vdW) interactions. It is planned to extend previous work of the group [1,2] towards a self-consistent treatment of non-local correlations leading also to vdW forces. Besides the adsorption geometry and energy, and the electronic structure [3] including level alignment, also the calculation of optical properties within TDDFT and/or manybody perturbation theory (the Bethe-Salpeter Equation) [4] will be of key interest.

Requirements:

We are looking for an outstanding PostDoc candidate who has an excellent theoretical background as well as experience in electronic structure calculations for complex materials. We offer a lively atmosphere in an international team working on various scientific topics. The position is part of an Austrian National Research Network (NFN) entitled „Interface controlled and functionalized organic molecules“ which requires close cooperation with the experimentalists of the consortium [3,4]. There will also be a strong link to the second theory PostDoc from this NFN within our group who will focus on the modeling of thin film growth of organic molecules [5].

Deadline:

February 28th, 2009

Contact:

Prof. Claudia Ambrosch-Draxl
Applications including CV and two letters of recommendation shall be sent by e-mail in PDF form to cad@unileoben.ac.at and peter.puschnig@unileoben.ac.at

References:

[1] P. Sony, P. Puschnig, D. Nabok, and C. Ambrosch-Draxl, Phys. Rev. Lett. 99, 176401 (2007).
[2] Dmitrii Nabok, Peter Puschnig, and Claudia Ambrosch-Draxl, Phys. Rev. B 77, 245316 (2008).
[3] G. Koller, S. Berkebile, M. Oehzelt, P. Puschnig, C. Ambrosch-Draxl, F. P. Netzer, and M. G. Ramsey, Science 317, 351 (2007).
[4] K. Hummer, P. Puschnig, and C. Ambrosch-Draxl, Phys. Rev. Lett. 92, 147402 (2004).
[5] G. Hlawacek, P. Puschnig, P. Frank, A. Winkler, C. Ambrosch-Draxl, and C. Teichert, Science 321, 108 (2008).