

## O 52: Methods: Atomic and Electronic Structure II

Time: Thursday 11:15–12:45

Location: H42

O 52.1 Thu 11:15 H42

**Electronic excitations and excited-state forces of the H:Si(001)-(2x1) monohydride surface** — NENG-PING WANG<sup>1</sup>, ●MICHAEL ROHLFING<sup>2</sup>, PETER KRÜGER<sup>3</sup>, and JOHANNES POLLMANN<sup>3</sup> — <sup>1</sup>Institut für Angewandte Physik und Zentrum für Mikrostrukturforschung, Universität Hamburg — <sup>2</sup>Fachbereich Physik, Universität Osnabrück — <sup>3</sup>Institut für Festkörpertheorie, Universität Münster

We investigate electronic excitations of the H:Si(001)-(2x1) monohydride surface using first principles approaches. Density-functional theory is used to calculate the ground state geometry of the system. The quasiparticle band structure is calculated within the *GW* approximation. Taking the electron-hole interaction into account, electron-hole pair states and optical excitations are obtained from the solution of the Bethe-Salpeter equation for the electron-hole two particle Green function. In this work we focus, in particular, on localized excitations of the silicon-hydrogen bonds at the surface layer. These excitations give rise to an outward-directed force on the hydrogen atoms, which may well explain their optically induced desorption from the surface as observed in recent experiments. The localization of the excitation is described by an artificial confinement potential in addition to standard many-body perturbation theory.

[1] N.-P. Wang, M. Rohlfing, P. Krüger, and J. Pollmann, *Phys. Rev. B* 74, 155405 (2006).

O 52.2 Thu 11:30 H42

**Towards excitation spectra for molecules on surfaces: quasiparticle energy calculations** — ●XINGUO REN, PATRICK RINKE, VOLKER BLUM, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut der MPG, D-14195, Berlin

To study adsorption-related changes in the electronic structure of molecules from first principles, it is highly desirable to have a computational scheme that can treat both confined (molecules) and extended systems (surfaces) efficiently on equal footing. For present-day excited-state formalisms, achieving this “equal footing” is a challenge. Based on a new highly efficient local-orbital DFT code [1], we have developed a local-orbital based formalism of the *GW* approximation for the many-body self-energy, allowing us to calculate the quasiparticle excitation energies of confined systems efficiently. Focussing on the description of isolated molecules we show for the example of benzene how different local exchange-correlation functionals (LDA, PBE) and non-local (hybrid) schemes (HF, PBE0) affect the atomic and electronic structures of the ground state. In a second step we demonstrate the influence of the ground state functional on the *GW* excitation spectrum and compare this to previous calculations [2].

[1] V. Blum, R. Gehrke, P. Havu, V. Havu, X. Ren, and M. Scheffler, *The FHI Ab Initio Molecular Simulations (AIMS) project*, Fritz-Haber-Institut, Berlin (2006).

[2] M.L. Tiago and J.R. Chelikowsky, *Solid State Commun.* **136**, 333 (2005).

O 52.3 Thu 11:45 H42

**Control of dissipative quantum systems** — ●ERIK ASPLUND and THORSTEN KLÜNER — Institute of Pure and Applied Chemistry, Carl v. Ossietzky University Oldenburg, Germany

Light interacting with atoms and molecules is not only a source of information about the atoms and molecules studied, it can also initiate charge and energy transfer processes, i.e. chemical reactions. The ability to control quantum systems interacting with their environment and light is investigated. A quantum system interacting with the environment can be separated into a primary system and a bath. This can be done within the framework of the Surrogate Hamiltonian approach [1]. Optimal control theory (OCT) provides a tool to active control of quantum dynamical systems [2]. To gain control of a dissipative system, OCT is combined with the Surrogate Hamiltonian method. It is shown that an effective control of a dissipative system is possible. Theoretical quantum calculations on the benchmark system NO/NiO(100) are provided to illustrate this combined approach and the results are compared with previous studies [3,4].

[1] Roi Baer, and Ronnie Kosloff, *J. Chem. Phys.* 106, 8862 (1997). [2] Wusheng Zhu, Jair Botina, and Herschel Rabitz, *J. Chem. Phys.* 108, 1953 (1997). [3] Christiane P. Koch, Thorsten Klüner, Hans-Joachim Freund, and Ronnie Kosloff, *J. Chem. Phys.* 119,1750 (2003).

[4] Sören Dittrich, Hans-Joachim Freund, Christiane P. Koch, Ronnie Kosloff, and Thorsten Klüner, *J. Chem. Phys.* 124, 024702 (2006).

O 52.4 Thu 12:00 H42

**Electron coincidence spectroscopy from surfaces: insulator vs. metal** — ●FRANK OLIVER SCHUMANN, CARSTEN WINKLER, and JÜRGEN KIRSCHNER — Max-Planck-Institut für Mikrostrukturphysik

The effect of electron correlation manifests itself in the creation of the exchange-correlation (xc) hole. This theoretical concept is an important part of modern solid state theory. We have shown previously that the xc-hole is experimentally accessible via electron pair emission from surfaces. In order to assure that the xc-hole can be fully mapped we devised a new time-of-flight set-up with large angular acceptance. This is achieved by means of three channelplate detectors with delay lines anodes. We demonstrate that the xc-hole can now be fully mapped and a material dependent study becomes feasible. This is of general interest for a deeper understanding of the electron-electron interaction. We report on the first experiment aiming to unravel the material dependence of the xc-hole. We compare a Cu(100) surface with an insulator like LiF(100) and find distinctive differences in the electron-electron interaction. The spatial extension of the xc-hole shows a larger size for Cu compared to LiF. We further find that the angular extension of the xc-hole is independent of the kinetic energy in both cases. For certain energies of the electrons the xc-hole vanishes. The origin of this behavior is connected to the 2D-energy distributions.

O 52.5 Thu 12:15 H42

**Spectro-Microscopy with very high resolution demonstrated at selected surface systems** — ●FLORIAN MAIER<sup>1</sup>, HELDER MARCHETTO<sup>2</sup>, ULRICH GROH<sup>1</sup>, PIERRE LEVESQUE<sup>2</sup>, TOMAS SKALA<sup>2</sup>, THOMAS SCHMIDT<sup>1</sup>, RAINER FINK<sup>3</sup>, HANS-JOACHIM FREUND<sup>2</sup>, EBERHARD UMBACH<sup>1</sup>, and THE SMART-COLLABORATION<sup>1,2,3,4</sup> — <sup>1</sup>Universität Würzburg, Experimentelle Physik II, 97074 Würzburg — <sup>2</sup>Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14159 Berlin — <sup>3</sup>Univ. Erlangen-Nürnberg, Phys. Chemie II, 91058 Germany — <sup>4</sup>TU Clausthal, TU Darmstadt, ZEISS Oberkochen, BESSY Berlin

The aberration corrected spectro-microscope SMART has been developed for all kinds of photo emission (PEEM) and low energy electron microscopy (LEEM) with outstanding lateral and energy resolution. The recent performance of the well operating instrument is shown, and the capabilities of spectroscopic imaging will be demonstrated for selected sample systems. We will especially concentrate on the adsorption behaviour of the organic molecule PTCDA(3,4,9,10-perylene-tetracarboxylic-acid dianhydride) on Ag(111) and Au(111) surfaces. For example, local work function, spectroscopic information, and even structural differences can be used for image contrast formation. This also allows correlating the substrate morphology with, e.g., the interaction with the organic molecules and even, by taking advantage of the high instrumental transmission, to observe directly, i.e. in real time and in situ, the growth of interface systems. (Funded by BMBF, contract 05KS4WWB/4)

O 52.6 Thu 12:30 H42

**Verification of Phase Retrieval Parameters by coherent Measurement itself** — ●T. PANZNER<sup>1</sup>, T. SANT<sup>1</sup>, G. GLEBER<sup>1</sup>, I. VARTANYANTS<sup>2</sup>, and U. PIETSCH<sup>1</sup> — <sup>1</sup>Festkörperphysik, Institut für Physik, Universität Siegen, Germany — <sup>2</sup>HASYLAB-DESY, Hamburg

Monochromatic scattering experiments using a coherent x-ray beam have shown the great potential to get access to atomic resolved results without special preparation of the sample. The big disadvantage of all scattering experiments is the loss of phase information of the scattered signal. Therefore, so called “phase retrieval” procedures are needed to restore the wanted information from the measured intensities. The quality of these procedures strongly depends on additional information about the illuminated area. This information can be given by the size of the illuminated area (“over sampling” [1]) or the illumination function itself (i.e. approximation by Fermi-integrals [2]). In our case (energy-dispersive set-up) we have shown, that the illumination function is well determined by the aperture (pinhole) being equipped in front of the sample. A simple FFT of a measured intensity map is sufficient to reproduce the calculated intensity distribution. The deviation of the reconstructed illumination function from the calculated

one, represents the influence of the specimen to the scattering intensity. In case of a reflectivity experiment this information concerns the roughness of surface. Our future work is concentrated on these varia-

tions to improve the quality of the phase retrieval procedure. [1] J. Miao et al, Phys. Rev. B 67, 174104 [2] I.A. Vartanyants et al, Phys. Rev. B 55, 13193