

O 41 Electronic structure III

Time: Thursday 15:00–17:30

Room: WIL B321

O 41.1 Thu 15:00 WIL B321

Focusing effect on surfaces due to scattering of bulk electrons at subsurface impurities — ●SAMIR LOUNIS, PHIVOS MAVROPOULOS, PETER H. DEDERICHS, and STEFAN BLÜGEL — Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany

An impurity placed below the surface of a noble metal acts as a scatterer of bulk electrons which can lead to short wavelength patterns at the surface as recently found in STM experiments [1]. As explained by these authors the scattering intensity is focused in special directions being determined by regions of low curvature on the Fermi surface. Motivated by this, we carried out a systematic theoretical investigation on the scattering effect of a Co impurity buried at different positions below the (001), (110) and (111) surfaces of noble metals. The wavelength patterns which are related to the curvature of the Fermi surface of the host have different shapes depending on the orientation of the surface. In addition we discuss typical anomalies arising from the reflection of the scattered waves at buried interfaces. The calculations were performed using the full-potential scalar-relativistic Korringa-Kohn-Rostoker Green-function method within Density Functional Theory.

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[1] A. Weismann, M. Wenderoth, N. Quaas, and R. G. Ulbrich, *Verhandlungen der Deutschen Physikalischen Gesellschaft*, O 36.13, 502 (2005) (unpublished).

O 41.2 Thu 15:15 WIL B321

Electronic structure of molybdenum dioxide. Periodic and cluster DFT quantum chemical studies. — ●RENATA TOKARZ-SOBIERAJ, MALGORZATA WITKO, and ROBERT GRYBOS — Institute of Catalysis and Surface Chemistry, PAS, Cracow, Poland

DFT method is used to describe the electronic structure of bulk and catalytically interesting (011) surface of molybdenum dioxide. MoO₂ exists in literature mainly as a product of MoO₃ reduction; however, the problem of its role in catalytic processes is still unsolved. The electronic structure of bulk system is calculated using periodic approach (VASP code), whereas the information of monoclinic (011) surface is obtained from the cluster method (StoBe code). In both calculations the gradient corrected functionals are used. Detailed analyses of total and atom projected density of states (DOS, PDOS) yield metallic behavior for MoO₂ bulk material. The band around the Fermi level is mainly of Mo 4d character, whereas directly below - there are the O 2p bands (up to -3eV). Further, below EF there is a band (from -3 to -8 eV) identified as Mo-O bonding molecular orbitals. Local properties of different surface sites that are exposed at (011) surface, namely five- and six- fold coordinated Mo atoms, and nucleophilic O sites with different coordination numbers are discussed using charge densities, bond orders indices and molecular orbital diagrams. The discussed surface is characterized by DOS spectra similar to the bulk. Pairs of metallic sites and isolated oxygen centers are identified.

O 41.3 Thu 15:30 WIL B321

Theoretical investigations of molecule-metal interfaces — ●LORENZ ROMANER^{1,2}, GEORG HEIMEL², PETER PACHER^{1,2}, MATHIS GRUBER^{1,2}, JEAN-LUC BRÉDAS², and EGBERT ZOJER^{1,2} — ¹Institute of Solid State Physics, Graz University of Technology, Petersgasse 16, A-8010 Graz, Austria. — ²School of Chemistry and Biochemistry and Center for Organic Photonics and Electronics, Georgia Institute of Technology, Atlanta, Georgia 30332-0400.

We present a theoretical investigation of π -conjugated molecules bound to metallic surfaces. The physical properties of organic/metal interfaces are of high interest for the understanding of self-assembled monolayer formation, workfunction modification of metals, injection barrier tuning in electronic devices, chemical sensing, and molecular electronics. By means of band-structure calculations based on density functional theory, we discuss the interplay between: i) the formation of the bond between metal atoms and atoms of the molecular docking groups; ii) the hybridization and alignment of the molecular states with the Bloch states of the metal; and iii) the charge redistribution between metal and molecule. To that purpose, we systematically varied the molecular structure by exchanging the docking groups, attaching different donor/acceptor groups

to the molecule and varying the conjugation length. We also analyze the reversal of interface formation by mechanically stretching a metal-molecule-metal structure and focusing on stretching forces and structural deformations.

O 41.4 Thu 15:45 WIL B321

Stability of different V2O5 surfaces - theoretical studies — ●MALGORZATA WITKO, JAKUB GOCLON, and ROBERT GRYBOS — Institute of Catalysis and Surface Chemistry, PAS, Cracow, Poland

Vanadia-based catalysts have a well established position both for large-scale applications and as laboratory research material. Experimental studies on vanadia crystallites point out the presence of only (010) surface. On the other hand, a wide spectrum of reactions, which are catalyzed by vanadia-based materials, suggests an important role of other low-index surfaces such as (001) and (100). Therefore, the relative stability of 3 stoichiometric surfaces (010), (100) and (001)V₂O₅ is studied and compared. Surface energy of low-index terminations is calculated using the periodic DFT approach employing the VASP code. V₂O₅ has a structure of weakly interacting layers stacked along [010] direction, therefore the (010) surface can be modeled by only one layer, whereas the (001) and (100) surfaces need models containing larger number of layers. It is found that the relative stability of surfaces changes in the following order: (010) > (001) > (100). For all surfaces, ionic positions are optimized. Only for the (001) surface a considerable energetic effect of relaxation is found. Surface free energies obtained from DFT calculations are used to make the Wulff construction for V₂O₅ crystal.

O 41.5 Thu 16:00 WIL B321

Reactivity of different V2O5 surfaces - cluster DFT studies — ●PAWEŁ HEJDUK¹, MALGORZATA WITKO¹, and KLAUS HERMANN² — ¹Institute of Catalysis and Surface Chemistry, PAS, Cracow, Poland — ²Fritz-Haber Institut der MPG, Berlin, Germany

The wide application of vanadium oxides as catalysts follows from the fact that their crystallites may exhibit two structurally different types of faces: surfaces built of chemically saturated atoms and those built of unsaturated cations and anions. Both show different behavior in catalytic reactions by performing a complex multi-step operation on the reacting molecule through activation of some of the reactant bonds and hindering those interactions which could result in unwanted product. In this study the reactivity of saturated (010) and unsaturated (001) and (100) surfaces is determined by ab initio DFT cluster methods where electron exchange and correlation is approximated by the gradient corrected RPBE functional. Detailed electronic structure analyses are performed using Mulliken populations and Mayer bond indices, electrostatic potentials, total and partial (atom projected) densities-of-states. Further, adsorption of one and two hydrogen atoms as an atomic/molecular probe at the different surfaces, which leads to surface OH and H₂O or two OH species, will be discussed in detail.

O 41.6 Thu 16:15 WIL B321

Coverage-dependent evolution of plasmon modes in adsorbed Cs layers on Si(111) — ●VOLKMAR ZIELASEK^{1,2}, NEELE RÖNITZ³, EDDY PATRICK RUGERAMIGABO¹, MARTIN HENZLER¹, and HERBERT PFNÜR¹ — ¹Universität Hannover, Institut für Festkörperphysik, Appelstr. 2, 30167 Hannover — ²Universität Bremen, Institut für Angewandte und Physikalische Chemie, Leobener Straße, NW II, 28359 Bremen — ³Philips Semiconductors, Stresemannallee 101, 22529 Hamburg

The transition between substrate and overlayer metalization with varying alkali metal coverage has been studied for Si(111) (7 × 7)-Cs by EELS with ultra-high momentum resolution and measurements of electrical conductance at low temperatures. As the Cs coverage is increased from 0.5 to 1.2 ML coverage, the predominant surface plasmon transforms from a monopole mode, representing metallicity in substrate surface states modified by Cs, to an overlayer multipole mode, which indicates metallicity within a Cs adlayer. The multipole mode continuously shifts in energy from 1.4 to 2.2 eV until a continuous Cs wetting layer is formed. In contrast to previous conventional EELS experiments, the multipole plasmon is clearly identified by an extremely narrow angular distribution of the inelastic electron scattering, unaccounted for by standard dipole scattering theory. Its observation provides evidence for luminescence from atomic Cs layers on Si(111) which can be tuned from infrared to the visible energy range by adjusting Cs coverage.

O 41.7 Thu 16:30 WIL B321

Quantum Size Effects in a decoupled Pb slab on graphitized SiC — •HUGO DIL¹, THORSTEN KAMPEN¹, THOMAS SEYLLER², and KARSTEN HORN¹ — ¹Department of Molecular Physics, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — ²Institute of Technical Physics, University of Erlangen-Nürnberg, Erwin-Rommel-Straße 1, 91058 Erlangen, Germany

Quantum size effects (QSE) which occur in metal overlayer when the dimensions become comparable to the de Broglie wavelength, are responsible for a wide variety of novel effects. In almost all previous work on this subject the influence of the substrate is not negligible. The preferred height of Pb layers on Si(111), for example, changes from 8 to 6 monolayers when depositing on either the 7x7 or sqrt3 x sqrt3. This can be either due to the interface atomic or electronic structure.

To study QSE in films decoupled from the substrate, one has to create a quasi free standing metal slab. We have accomplished this by depositing lead at low temperature on a single domain graphite substrate which shows very little interaction with the metal film. This substrate was prepared, according to a recently developed procedure, from H-etched SiC. The measured band structure of the Pb quantum well states shows an almost perfect match to density functional theory calculations for free standing lead slabs. The observed heights corresponds well to those expected from a simple total energy minimization principle.

O 41.8 Thu 16:45 WIL B321

Unusual temperature dependence of the surface state lifetime on Al(001) — •M. F. JENSEN¹, T. K. KIM¹, S. BENGIÒ¹, PH. HOFMANN¹, I. YU. SKLYADNEVA², A. LEONARDO², and E. V. CHULKOV² — ¹Institute for Storage Ring Facilities and iNano Center, University of Aarhus, 8000 Aarhus C, Denmark — ²Donostia International Physics Center (DIPC), 20018 San Sebastián / Donostia, Basque Country, Spain

The influence of many-body effects on surface state lifetimes, and in particular the role of the electron-phonon coupling, has recently attracted considerable attention. For temperatures higher than the surface Debye temperature, the situation is expected to be very simple: The inverse surface state lifetime depends linearly on the temperature with the slope mainly given by the electron-phonon mass enhancement parameter λ . Here we present results for the surface state on Al(001) which turns out to behave differently: for high temperatures a stronger than linear increase of the inverse lifetime is observed. The experimental results are compared to first-principles calculations and possible reasons for the unexpected temperature dependence are discussed.

O 41.9 Thu 17:00 WIL B321

Ab initio study of non-reconstructed clean and H-passivated SiC(0001) surfaces — •TASSILO DANNECKER, ALEXANDER MATTAUSCH, and OLEG PANKRATOV — Theoretische Festkörperphysik, Staudtstr. 7, 91058 Erlangen

The SiC(0001) surface is regarded as a two-dimensional Mott-Hubbard insulator [1]. Up to now mostly the reconstructed $\sqrt{3} \times \sqrt{3}R30^\circ$ -surface has been studied, whereas the 1×1 -surface was considered as unstable. However, recently the 1×1 -structure was stabilized by H-passivation. Moreover, after the hydrogen removal the surface remains metastable [2]. Early DFT-LDA calculations suggested a metallic character of both 1×1 - and $\sqrt{3} \times \sqrt{3}R30^\circ$ -surfaces [3]. However, experimentally the surfaces are semiconducting. For the $\sqrt{3} \times \sqrt{3}R30^\circ$ -surface it was suggested that the Hubbard correlations are responsible for its semiconducting state [1]. In this work we focus on the Si-terminated (0001) as well as the C-terminated (000 $\bar{1}$) side. We consider both clean and H-passivated surfaces. In particular, we study the nature of the surface electron states and in case of the H-passivated surface we discuss the resonant surface states, which are induced by the hydrogen-surface interaction.

[1] V.I. Anisimov *et al.*, Phys. Rev. B, **61** (2000) 1752.

[2] T. Seyller, J. Phys.: Condens. Matter, **16** (2004) 1755.

[3] M. Sabisch, P. Krüger and J. Pollmann, Phys. Rev. B **55** (1997) 10561.

O 41.10 Thu 17:15 WIL B321

Scattering of electrons in image-potential bands on Cu(001) by Co-Adatoms — •MICHAELA HIRSCHMANN, KLAUS BOGER, and THOMAS FAUSTER — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

Energy-, time- and angle-resolved two-photon photoemission has been used to study the various scattering processes induced by adsorbate atoms. We have examined the dynamics of electrons in image-potential

states on the Cu(001) surface covered by statistically distributed Co-Adatoms.

From the measured data the scattering probabilities of the inelastic and quasielastic, interband and intraband scattering processes can be determined. The results are discussed in relation to previous work for Cu on Cu(001) [1,2].

[1] K. Boger, M. Weinelt, Th. Fauster, Phys. Rev. Lett. **92** (2004) 126803

[2] K. Boger, Th. Fauster, M. Weinelt, New J. Phys. **7** (2005) 110