

O 25: Surfaces and films: forces, structure and manipulation

Time: Tuesday 15:00–16:15

Location: SCH A118

O 25.1 Tue 15:00 SCH A118

Understanding surface energies of transition metals with density-functional theory — ●ALOYSIUS SOON, MARTIN FUCHS, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut der MPG, Berlin, Germany

Determining index-specific surface energies of metals is, to date, still a non-trivial task, both experimentally and theoretically. Density-functional theory (DFT) calculations within the local-density approximation (LDA) for exchange-correlation (XC) have provided understanding of qualitative trends. Yet, absolute surface energies, in particular of *d*-metals still exhibit significant uncertainties related to the description of XC: gradient corrected functionals (GGA) which improve over the LDA for other properties often predict less accurate surface energies. This calls for a careful (re-)analysis of XC effects on surface energies, including non-local exchange and/or correlation.

Here we analyze the surface energies of 4*d*-metals with modern GGA functionals (PBEsol, AM05, developed to better describe bulk solids and (jellium) surfaces than the LDA and previous GGAs), using the all-electron FHI-aims code.¹ Relating the bulk cohesive energy and surface energy via a bond-cutting model we find that the modern GGAs can indeed correct the poorer results of the usual PBE-GGA but worsen the bulk cohesive energies of 4*d*-metals. In addition, we consider hybrid XC functionals (B3LYP, PBE0, and HSE03), using a cluster correction scheme,² and discuss the effects of including exact exchange on the calculated surface energies. 1. <http://www.fhi-berlin.mpg.de/aims/>; 2. Q.-M. Hu *et al.*, Phys. Rev. Lett. **98**, 176103 (2007); **99**, 169903(E).

O 25.2 Tue 15:15 SCH A118

Energetics, electronic structure, and packing density of the Ir, Pt, and Au(100) surface reconstructions by all-electron DFT — ●PAULA HAVU¹, VILLE HAVU¹, PATRICK RINKE^{1,2}, VOLKER BLUM¹, and MATTHIAS SCHEFFLER^{1,2} — ¹Fritz-Haber-Institut der Max-Planck-Gesellschaft, D-14195 Berlin, Germany — ²University of California at Santa Barbara, CA 93106, USA

Among fcc metals, only the late-5*d* transition metals Ir, Pt, and Au rearrange by quasihexagonal reconstructions on the nominally quadratic (100) surface structure. However, Ir reconstructs in one direction only [(5×1)], while Au(100) and Pt(100) rearrange in *both* lateral directions with large unit cells, often characterized as (5×*N*) (*N* ≥ 20 in the experimental literature). Elucidating the exact packing density and energetics have been the focus of many experiments, but theory has so far been relegated to either (5×1) approximants, or simplified empirical potentials. Using *N* = 1, 10, 15, 20, 25, 30 supercell models (up to 786 atoms/cell) and the FHI-aims code [1], we here show how all-electron density-functional theory (DFT) captures the energetics, electronic structure, and lateral packing densities of all three surfaces for different local-density and generalized gradient approximations. Remarkably, the effect of the 2D reconstruction [(5×*N*) instead of (5×1)] on the surface energy is nearly an order of magnitude bigger for Au than for Pt. DFT captures quantitatively the energetically rather subtle difference in packing densities, which is slightly higher for Au than Pt, consistent with experiment [2]. [1] V. Blum *et al.*, Comp. Phys. Comm., accepted (2008). [2] V. Jahns *et al.*, Surf. Sci. **430**, 55 (1999).

O 25.3 Tue 15:30 SCH A118

Melting of two-dimensional adatom superlattices stabilized by long-range electronic interactions — ●N. N. NEGULYAEV¹, V. S. STEPANYUK², L. NIEBERGALL², P. BRUNO^{2,3}, M. PIVETTA⁴, M. TERNES^{4,5}, F. PATTHEY⁴, and W.-D. SCHNEIDER⁴ — ¹Fachbereich Physik, Martin-Luther-Universität, D06099 Halle, Germany — ²Max-Planck-Institut für Mikrostrukturphysik, D06120 Halle, Germany — ³European Synchrotron Radiation Facility, F38043 Grenoble, France — ⁴Ecole Polytechnique Federale de Lausanne, CH1015 Lausanne, Switzerland — ⁵IBM Research Division, Almaden Research Center, San Jose, CA 95120, USA

According to the KTHNY theory [1], a true 2D solid melts to liquid

via intermediate phase, named hexatic.

Here we report on a combined experimental and theoretical study of the solid to liquid phase transition of 2D Ce adatom superlattices on Cu(111) and Ag(111) noble metal surfaces. Variable temperature STM measurements and DFT calculations elucidate the formation of the Ce superlattice, while kinetic Monte Carlo simulations describe the temperature dependent Ce adatom coordination within this 2D system [2]. Although the Ce superlattice is stabilized by long-range interactions mediated by surface-state electrons, the substrate atomic potential hinders the existence of the hexatic phase [2]. These results are in agreement with the melting behavior of a 2D lattice in the presence of a 'fine mesh' substrate potential [1].

[1] D.R. Nelson and B.I. Halperin, Phys. Rev. B **19**, 2457 (1979).

[2] N.N. Negulyaev *et al.*, Phys. Rev. Lett., submitted.

O 25.4 Tue 15:45 SCH A118

Second order phase transition and critical fluctuations in a quasi-1D system: Br/Pt(110) — ●MICHAEL CORDIN¹, BARBARA LECHNER¹, ALEXANDER MENZEL¹, ERMALD BERTEL¹, CESARE FRANCHINI², RAINALDO ZUCCA², and JOSEPH REDINGER² — ¹Institute for Physical Chemistry, University of Innsbruck, Austria — ²Center for Computational Materials Science, Vienna University of Technology, Austria

Deposition of 0.5 monolayers (ML) of Bromine on Pt(110) results in a c(2x2)-Br/Pt(110) structure with almost perfect long-range order at 300 K. Upon cooling this structure to 50 K a reversible, apparent "inverse" order-disorder transition is observed. On a nearly defect-free surface the c(2x2) structure decays into striped c(2x2) and (2x1) domains. The resulting stripe pattern exhibits typical hallmarks of critical behaviour, i.e. a scale-free domains-in-domains structure. We therefore conclude that there is a continuous phase transition between the (2x1) and the c(2x2) structure and the disorder at 50 K is due to the proximity of the critical temperature. The conclusion is supported by DFT calculations, which place the (2x1) as the stable groundstate 17 meV below the c(2x2) structure (at 0 K). Even very small defect concentrations lead to the appearance of a third structural element at 50 K, namely a local (3x2) unit mesh[1]. Possible origins of the continuous phase transition will be discussed.

[1] E. Dona *et al.*, Phys. Rev. Lett. **98**, 186101 (2007).

O 25.5 Tue 16:00 SCH A118

Surface reconstruction of clean bcc-Fe{110}: a quasi-hexagonal top-layer with periodic height modulation — ●TOYO KAZU YAMADA^{1,2}, HIDETOSHI TAMURA², MOTOYUKI SHISHIDO², TOSHIKAZU IRISAWA², LUKAS GERHARD¹, WULF WULFHEKEL¹, and TADASHI MIZOGUCHI² — ¹Physikalisches Institut, Universität Karlsruhe, Wolfgang-Gaede-Straße 1, 76131 Karlsruhe, Germany — ²Faculty of Science, Gakushuin University, 1-5-1 Mejiro, Toshima 171-8588, Tokyo, Japan

In general every surface has stress due to a symmetry break. When the stress overcomes the elastic limit, the surface reconstructs. There have been found surface reconstructions on only several metal surfaces. So far, no surface reconstruction was reported on the Fe surface. Iron is an important popular ferromagnetic metal which has been widely used since the ancient age in practical applications owing to its strength and abundance. We use Fe single crystals made by a chemical vapor deposition technique, which include no impurities in bulk and give us an extremely clean surface.

We found a new surface reconstruction on the {110} plane of bcc Fe-whisker single crystals. Atomically-resolved STM images showed a quasi-hexagonal atomic array with mesoscopic-range periodic height modulation of about 1/3 of an atomic step. This height modulation was found to be a result of an interference between the quasi-hexagonal top-layer and the sub-surface bcc-Fe{110} layer. Details of the atomic structure as well as local density of states of this new reconstruction are presented.