

fail to yield a converged lattice constant perpendicular to the graphene sheets[1].

Therefore we investigate the influence of an additional long-range attractive term based on the London description of van der Waals forces[2]. It is found that one obtains the correct c lattice constant of graphite while the changes of the bulk properties of diamond due to the inclusion of the van der Waals term are negligible. Results for the relaxation of the graphite surface will be presented.

[1] K. R. Kganyago and P. E. Ngoepe, *Molecular Simulation* **29**, 39 (1999)

[2] F. London, *Z. Phys. Chem. Abt. B11*, 222 (1930)

O 36.77 Mo 15:00 Poster TU F

DFT studies of charged gold surfaces — ●MARTINA NOTHACKER¹, FERDINAND EVERS¹, KLAUS-PETER BOHNEN², ROLF HEID², FLORIAN WEIGEND¹, CHRISTIAN ELSÄSSER³, and JÖRG WEISSMÜLLER¹ — ¹Institut für Nanotechnologie, Forschungszentrum Karlsruhe, 76021 Karlsruhe, Germany — ²Institut für Festkörperphysik, Forschungszentrum Karlsruhe, 76021 Karlsruhe, Germany — ³Fraunhofer Institut für Angewandte Festkörperphysik, 79108 Freiburg, Germany

The study of surface and interface properties, electronic and structural, has a long history. Surprisingly, very little is known about the change of these properties, for instance in bandstructure, surface atom configuration etc. when the surface is being charged. In view of recent experiments, we use density functional methods in order to analyze how the reconstruction of a planar gold surface is modified with increasing surface excess charge. Our results for the planar surface will be compared to data for charged gold clusters, where we find a behavior in qualitative agreement with the experimental findings.

O 36.78 Mo 15:00 Poster TU F

The aqueous-solution gas interface of sodium halogenides — ●MICHAEL PAULUS¹, CHRISTIAN GUTT¹, MICHAEL SPRUNG², CHRISTOPH KRYWKA¹, and METIN TOLAN¹ — ¹Experimentelle Physik I, Universität Dortmund, Maria-Goeppert-Mayer Str. 2, 44227 Dortmund, Deutschland — ²c/o SID/IMMY-XOR-CAT, APS/ANL, Argonne, IL, 60439, USA

We present an in-situ grazing incidence diffraction (GID) experiment to study the aqueous-solution gas interface of the sodium halogenides, NaCl, NaBr and NaI. The aim of our experiment was to investigate the microscopic structure of the aqueous-solution gas interface and its changes for different types of salt in comparison with a water surface. Besides the appearance of the ion structure factor we observe a reduction of the surface energy at short length scales as it was calculated by Mecke et al PRE 59 (6) 6766 (1999).

O 36.79 Mo 15:00 Poster TU F

Dynamics of ice surface morphologies close to the melting point — ●SEBASTIAN SCHÖDER, HARALD REICHERT, SIMON ENGEMANN, and HELMUT DOSCH — Max-Planck-Institut für Metallforschung, Heisenbergstrasse 3, D-70569 Stuttgart

Ice surfaces play an important role in many natural and technical systems. In order to get access to the dynamics of ice surface structures, we have investigated a vicinal ice surface. The dynamics of the facets was examined with dynamic light scattering in a specially designed experimental chamber. This setup allows us to accurately control the sublimation rate of the observed surface. The results were compared for different temperatures. For low temperatures (-12.5 degrees) no dynamics was found. For temperatures close to the melting point we found dynamic correlations with a correlation time in the order of ten minutes. We attribute this temperature dependent behaviour to the surface melting of ice.

O 37 Hauptvortrag Soukiassian

Zeit: Dienstag 09:45–10:30

Raum: TU EB301

Hauptvortrag

O 37.1 Di 09:45 TU EB301

Silicon Carbide Surfaces: Metallization versus Passivation — ●PATRICK SOUKIASSIAN — Commissariat à l'Energie Atomique, Laboratoire SIMA associé à l'Université de Paris-Sud/Orsay, DSM-DRECAM-SPCSI, Saclay, Bâtiment 462, 91191 Gif sur Yvette Cedex, France

Silicon carbide (SiC) is an advanced semiconductor especially promising in high power, high temperature, high voltage and high frequency micro-electronics devices and sensors. Cubic and hexagonal SiC surfaces exhibit many reconstructions (over 10). SiC nanochemistry with oxygen and hydrogen is studied by atom-resolved scanning tunneling microscopy and spectroscopy, synchrotron radiation based- core level and valence band photoemission spectroscopies, and infrared absorption spectroscopy. The following results will be presented and discussed: i) Atomic

scale understanding of O₂ interaction and initial oxide interface formation. ii) The first example of H-induced semiconductor surface metallization. This unprecedented behavior results from H-creating a specific defect coming from competition between hydrogen termination of surface dangling bonds and hydrogen-generated steric hindrance below the surface. In addition, such a H-induced metallization is not removed by oxygen exposures and most interestingly, also takes place on a pre-oxidized SiC surface. This H-induced metallization directly impacts the ability to eliminate electronic defects at semiconductor interfaces critical for microelectronics, provides means to develop electrical contacts on high band-gap chemically passive materials, particularly exciting for interfacing with biological systems where oxygen is unavoidable, and gives control of surfaces for lubrication, e.g. in nanomechanical devices.

O 38 Halbleiteroberflächen und -grenzflächen

Zeit: Dienstag 10:45–13:00

Raum: TU EB301

O 38.1 Di 10:45 TU EB301

Atomic structure of the GaAs(001)- $c(4 \times 4)$ surface: first-principles evidence for diversity of heterodimer motifs — ●E. PENEV^{1,2}, P. KRATZER¹, and M. SCHEFFLER¹ — ¹Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4–6, D-14195 Berlin — ²Institut für Physik, Universität Basel, CH-4056 Basel, Schweiz

The atomic structure of the $c(4 \times 4)$ reconstruction, formed on the GaAs(001) surface under high arsenic overpressure, has recently been attracting renewed interest. This has led to a revision of the commonly accepted $c(4 \times 4)$ structural model but a definitive understanding of the driving force for the newly proposed structure[1] was lacking. Targeting the later problem, the talk will present a state-of-the-art theoretical study of the GaAs(001)- $c(4 \times 4)$ surface employing *ab initio* atomistic thermody-

namics based on density-functional theory calculations. We shall demonstrate[2] that in a range of stoichiometries, between those of the conventional three As-dimer and the new three Ga-As dimer model[1], there exists a diversity of atomic structures featuring Ga-As heterodimers, driven by surface configurational entropy. These results fully explain the experimental scanning tunneling microscopy images and are likely to be relevant also to the $c(4 \times 4)$ -reconstructed (001) surfaces of other III-V semiconductors.

[1] A. Ohtake *et al.*, *Phys. Rev. Lett.* **89**, 206102 (2002).

[2] E. Penev *et al.*, *Phys. Rev. Lett.* **93**, 146102 (2004).