

O 32 Adsorption IV

Time: Thursday 11:15–13:00

Room: TRE Phys

O 32.1 Thu 11:15 TRE Phys

Organic molecules on surfaces: Structural and dynamical properties — ●MARTIN PREUSS¹, KAORI SEINO¹, WOLF GERO SCHMIDT², and FRIEDHELM BECHSTEDT¹ — ¹Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Germany — ²Fakultät für Naturwissenschaften, Department Physik, Universität Paderborn, Germany

For the microscopic control of organically functionalized surfaces an understanding on the atomic scale can only be achieved by combined experimental and theoretical studies. For the elucidation of interface structures infrared (IR) and high-resolution electron energy loss spectroscopy (HREELS) are among the most prominent methods due to the sensitivity towards subtle changes in geometry and, hence, vibrational properties. The determination of normal-mode and phonon frequencies belongs to the standard repertoire of density-functional theory (DFT) calculations whereas the corresponding intensities are seldomly reported. We have recently implemented a simple but accurate method into an existing plane-wave DFT code that allows for the calculation of the dynamical dipoles, and thus of IR intensities, for extended systems. For test purposes, the procedure is applied to small isolated molecules (NH₃, AlH₃, H₂O) and to benzene (C₆H₆) adsorbed on the Si(001) surface. For the system of perylene (C₂₀H₁₂) on Si(001) studied lately we scrutinize a number of possible adsorption configurations and single out the most probable one by comparison of the calculated and the measured vibrational spectrum.

O 32.2 Thu 11:30 TRE Phys

Observation of the Dynamical Change in a Water Monolayer Adsorbed on a ZnO Surface — ●B. MEYER¹, O. DULUB², and U. DIEBOLD² — ¹Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum — ²Department of Physics, Tulane University, New Orleans, USA

A combined density functional theory (DFT) and scanning tunneling microscopy (STM) study shows a rich structure of water monolayers adsorbed on the ZnO(1010) surface at room temperature. Most of the water is in a lowest-energy configuration where every second molecule is dissociated. It co-exists with an energetically almost degenerate configuration, consisting of a fully molecular water monolayer. Parts of the layer continuously switch back and forth between these two states. DFT calculations reveal that water molecules repeatedly associate and dissociate in this sustained dynamical process.

[1] O. Dulub, B. Meyer, U. Diebold, Phys. Rev. Lett. **95**, 136101 (2005)

O 32.3 Thu 11:45 TRE Phys

Wetting behavior of low-index cubic SiC surfaces — ●ALESSANDRA CATELLANI¹, GIANCARLO CICERO^{2,3}, and GIULIA GALLI³ — ¹CNR-IMEM, Parco Area delle Scienze 37a, I-43010 Parma, Italy — ²Physics Department, Torino Polytechnic, C. Duca degli Abruzzi, 24, I-10129 Torino, Italy — ³Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, California 94550, USA

We report on the interaction of water molecules with polar and non polar stoichiometric surfaces of cubic silicon carbide, as described by ab initio molecular dynamics at finite temperature. Our calculations show that, irrespective of coverage, in the gas phase water spontaneously dissociates on both polar Si-terminated (001) and non-polar (110) surfaces, following similar mechanisms. The specific geometric arrangement of atoms on the outermost surface layer is responsible for water orientation and coordination and thus plays a major role in determining surface reactivity. The ability of the crystalline surfaces with different polarity to induce water dissociation can be related to the similarities of their ionization potentials.

O 32.4 Thu 12:00 TRE Phys

Ab initio study of chemisorption reaction of Carboxylic group on Hydrogenated Silicon — ●ALESSANDRA CATELLANI^{1,2}, CLOTILDE S. CUCINOTTA^{2,3}, ALICE RUINI^{2,3}, MARILIA J. CALDAS^{4,2}, and ELISA MOLINARI^{2,3} — ¹CNR-IMEM, Parco Area delle Scienze 37a, 43010 Parma, Italy — ²CNR-INFN National Center on nanoStructures and bioSystems at Surfaces (S3), Via Campi 213a, 41100 Modena, Italy — ³Dipartimento di Fisica, Università di Modena e Reggio Emilia, Via Campi 213a, 41100 Modena, Italy — ⁴Instituto de Fisica, Universidade de Sao Paulo, Cidade Universitaria, 05508-900 Sao Paulo, Brazil

We studied the reactivity of the dihydrogenated Si(001) surface exposed to propionic acid [1]. The NEB method has been applied to predict energy barriers for chemisorption through the diverse O atoms pertaining to the -COOH group; the different paths to double Si-O bond formation are compared, and discussed in the light of grafting probability and functionalization stability.

[1] C. S. Cucinotta, A. Ruini, M. J. Caldas, and E. Molinari, J. Phys. Chem. B **108**, 17278 (2004).

O 32.5 Thu 12:15 TRE Phys

Conformational changes in adsorbed molecules — ●PHILIPP MARTIN SCHMIDT, THORSTEN U. KAMPEN, J. HUGO DIL, and KARSTEN HORN — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

Stilbene is the monomer building block of phenylenevinylene-type oligomers and polymers. It undergoes an interconversion around the central C=C double bond upon irradiation with UV-light of 250-320nm wavelength. This cis-trans-isomerization of the free molecule follows an in-plane hula-twist mechanism whose pathway can be assumed to work also in constraint systems as on surfaces - thus assessing a 'molecular switch'. To investigate the isomerization of stilbene-molecules on surfaces, planar trans(t)-stilbene has been studied on Si(100) surfaces at ~90 K by means of UPS and NEXAFS. Valence band spectra show that t-stilbene adsorbs undissociated onto the Si(100) surface. Neither Si2p nor C1s core level spectra show an energy shift upon coverage of the surface with t-stilbene, suggesting that the interaction is weak. Intensity changes of different components of the Si2p and C1s reveal that bonding takes place between Si dimers and the carbon atoms in the central C=C double bond. NEXAFS spectra indicate that the first layer of t-stilbene adsorbs in a flat orientation with the benzene rings being parallel to the substrate surface. Multilayers, on the other hand, physisorb highly disordered. A comparison of valence band spectra of trans- with cis-stilbene reveal significant differences which may permit an identification of both isomers for a further investigation of the isomerization process.

O 32.6 Thu 12:30 TRE Phys

Nano-ordering of defect structures in disordered Au/Si(111)-(5x2) — ●CHRISTOPH SEIFERT, CHRISTIAN WIETHOFF, FRANK MEYER ZU HERINGDORF, and MICHAEL HORN-VON HOEGEN — Universität Duisburg-Essen, Duisburg, Germany

Au adsorption at elevated temperatures in the Au coverage regime of up to 0.4 ML on Si(111) leads to the formation of (5x2) reconstructed domains. The electron diffraction pattern of this surface resembles that of a (5x1) reconstructed surface with additional pronounced lines at 50% Brillouin-Zone. These lines are well known to be caused by a random phase-shift of adjacent rows of the reconstruction in the two-fold direction [1].

Preparation at temperatures above 500°C - in combination with an increased Au coverage - yields a pronounced wavy modulation of these lines with a 20% BZ periodicity, which is visible after cool-down to room-temperature. This modulation is caused by an ordering of neighbouring phase-shifts and thus of the antiphase translational domains as well. A simple model, that qualitatively explains the resulting electron diffraction pattern, will be presented.

[1] Lipson et al. J. Phys. C **7**, p.12 (1974)

O 32.7 Thu 12:45 TRE Phys

Friction and adhesion mechanisms of the hairy attachment systems in spiders — ●MICHAEL SCHUCH¹, WOLFRAM HILD¹, KATHRIN CARL², YONGHE LIU¹, MATTHIAS SCHERGE³, and JUERGEN A. SCHAEFER¹ — ¹TU Ilmenau, Institut für Physik und Zentrum für Mikro- und Nanotechnologien, Postfach 100565, 98684 Ilmenau, Germany — ²TU Ilmenau, Fakultät für Maschinenbau, Postfach 100565, 98684 Ilmenau, Germany — ³IAVF Antriebstechnik AG, Im Schlehert 32, 76187 Karlsruhe, Germany

Biological attachment systems, such as the foot of geckos and spiders show a rich variety of shape and structure. Easy deformable attachment pads, hierarchical hairy structures with dimensions in the range of some hundred nm up to some μm lead to an enormous attachment ability. It has been proposed that attachment is achieved by the interaction between the attachment system and substrate, and by visco-elastic deformation. Both mechanisms are closely related with the contact area, which changes in the motion process. This work examines the contact area of spider feet on glass substrate and measures the friction and detachment forces. A living spider moving on a transparent glass substrate is observed by an optical microscope directly. The motion process recorded by a CCD-camera is examined to determine how the attachment and detachment are related with contact area of the spider feet. The foot prints obtained by a dying method are observed by a scanning electron microscope and correlated with the optical observations. Friction and detachment forces are measured with a microtribometer. The relationship between the friction and detachment forces and the contact area is discussed.