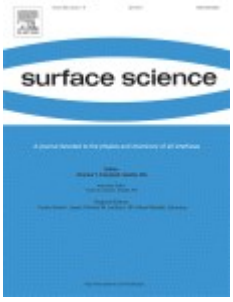

Surface Science

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Research Highlights

► One-dimensional dangling-bond wires fabricated on C(001), Si(001), and Ge(001) surfaces. ► Peierls instability or spin ordering in one-dimensional wires. ► The C wire has an antiferromagnetic spin ordering. ► The Ge wire has a Peierls-like lattice distortion.

Research Highlights

► Adsorption and desorption of fullerene on single-layer graphene. ► No modification of the band structure of graphene by fullerene. ► Use of fullerene as protection layer of graphene.

Research Highlights

► First structural characterization of buried nanoparticles by MEIS analysis. ► Mean size and number density of the Pb nanoparticles system were determined. ► No accurate information on the nanoparticle geometrical shape for the studied system.

Research Highlights

► Metallic character of thin Bi films on graphite was confirmed. ► Layer-pairing was observed. ► Deviations from the bulk atomic arrangement was identified. ► Presence of the second fast growth direction was indicated. ► Atomic resolution images were acquired.

Research highlights

► Formation of Au nanostructures on the rutile TiO_2(110) with different degree of O reduction. ► Au atoms adsorb strongest at oxygen vacancy sites. ► Potential energy profiles of the adsorbed Au monomers and dimers. ► Stable structures of different shape of two to nine Au atoms were determined. ► Infinitely long Au rows most stable of all investigated structures on the reconstructed TiO_2(110).

Research Highlights

► Au nanocrystals were probed with low energy alkali ion scattering. ► Au nanoclusters were deposited onto various Si oxide surfaces. ► The nanoclusters evolve from single layer to multilayer structures during growth. ► The nanoclusters display quantum effects as their size changes.

Research Highlights

► Alloying Fe and Co changes in preferable metal for CO adsorption. ► CO preferentially adsorbs on the Co-site of the FeCo alloys rather than the Fe-site. ► FeCo(100) is more reactive than pure Fe or Co surface due to lower work function. ► d-band center of Co atoms in FeCo alloy moves closer to Fermi level. ► d-band center of Fe atoms in FeCo alloy moves away from the Fermi level.

Research Highlights

► Ab initio path integral molecular dynamics simulations of hydrogen and deuterium adsorbed on/in the Pd(100) surface is reported. ► Significant quantum nuclear effects are found by comparing with conventional ab initio molecular dynamics simulations with classical nuclei. ► Ab initio path integral molecular dynamics simulations of surface and subsurface adsorption are now feasible.

Research Highlights

► A stable structure of clean GaN(0001) surface posses (2×1) reconstruction, having every second row of Ga located near plane of N atoms. ► Ga-related dispersionless surface electronic state was obtained, already identified by angle resolved photoelectron spectroscopy. ► For the adsorbate density up to one H atom for each Ga surface atom, the adatoms are located at the on-top positions. ► The H-related quantum surface state is located at valence band maximum (VBM) and deeply in the valence band, about 2 eV below VBM for p- and n-GaN surface, respectively which is related to Surface States Stark Effect (SSSE).

Research Highlights

► Extensive search for ground-state structures of the reduced SnO_2-(110) surface. ► Completion of the previously unknown equilibrium surface phase diagram. ► Proposal of a meta-stable surface reconstruction of the SnO_2-(110) surface. ► Assessment of the stability of meta-stable (4 × 1) reconstructions. ► Discussion of expected STM contrast on the basis of Tersoff–Haman calculations.

Research Highlights

► We consider the population of Rydberg states of ions escaping solid surfaces. ► We examine the resonances in probability distributions for multiply charged ions. ► The ionic core polarization strongly influences the final distributions. ► The argon anomaly is obtained within the two-state vector model.

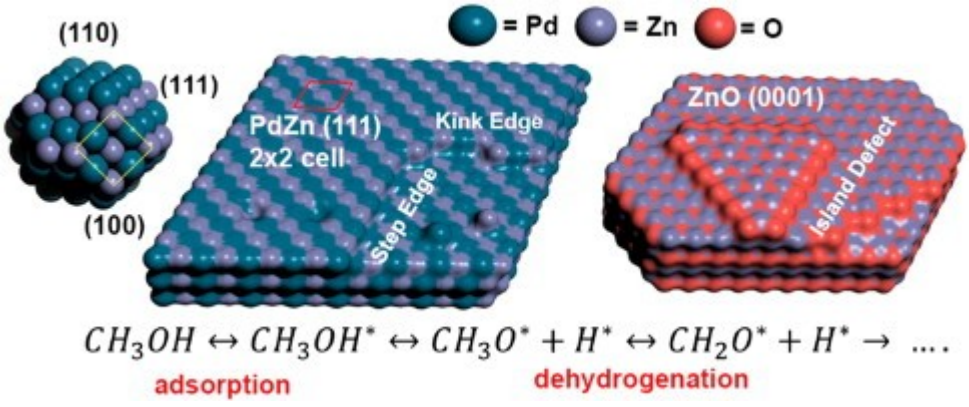
Research Highlights

► Properties of low index rutile TiO_2 surfaces. ► A new Tight-Binding Variable-Charge model for iono-covalent compounds. ► DFT calculations. ► Surface energies, atomic relaxations and charge transfer.

Research Highlights

► Benchmarking various dispersion correction schemes (DFT-D, vdW-DF, MP2) at noble gas dimers. ► Microscopic picture of the methane adsorption on graphene. ► Results fit experimental findings.

Graphical abstract



Research highlights

►CH_3OH and H_2O dissociations on defect-free PdZn surfaces are highly activated. ►Defects on PdZn surfaces lower these barriers. ►CH_3OH and H_2O dissociations on the ZnO(0001) surface have relatively low barriers.

Research Highlights

► Glycine adsorbs on Ge(100) − 2 × 1 by O–H dissociation. ► Major products are O-H dissociated adducts with some exhibiting N dative bonding. ► Minor product is dual O–H and N–H dissociated adduct. ► Coverage dependent product distribution is observed.

Research Highlights

►We calculate the electric conductances of atomic contacts consisting of Au, Al and Pt based on nonequilibrium Green's function theory and phase shift analysis. ►We analytically introduce the charge neutrality condition through the Friedel sum rule. ►We have analytically shown that the electric conductances are quantized and can increase when the distance between two electrodes increases. ►We conclude that the increment of the electric conductance is interpreted by the Friedel sum rule.

Research Highlights

► Reducing the band gap width of TiOx–Ny thin films. ► N-doped TiO_2. ► Reducing the surface energy. ► Hydrophobic properties. ► Selective optical coatings.

Research Highlights

► The amount of iron mass residual was inversely proportional to the wear rate. ► The

Research Highlights

► Angle-resolved inverse photoemission is performed on hydrogen-etched 6H-SiC(0001). ► Etching leads to silicate adlayer on SiC surface. ► No unoccupied Mott-Hubbard surface state observed after flashing samples. ► Saturation of dangling bonds by hydroxyl groups more likely than by hydrogen atoms.

Research Highlights

► Transition temperature of a 2D liquid phase of ethylbenzene was determined. ► Roles of the 2D liquid and substrate in finite-size effects on Tg were clarified. ► Quenching of crystallization from thin liquid films was observed.

Research Highlights

► The effect of boron doping Si nanocrystals on deuterium desorption is reported. ► A hot wire filament is used to dissociated D_2 to D and B_2D_6 to BD_x. ► Deuterium passivates Si dangling bonds and unreconstructs the surface dimer bonds. ► Boron backbonds with the silicon surface atoms and the next layer of silicon. ► The boron enhances nonradiative Auger recombination and quenches photoluminescence.

Research Highlights

► Finding a tilted off-top adsorption state for NH_3 on Ir(110). ► Presenting a micro picture for NH_3 decomposition. ► Revealing the main factors which influence NH_3 decomposition.

Research highlights

► HT CO-desorption from TiO_2 + Rh + CO_{sat} corresponds to C+O reaction on the titania support. ► Lack of CO_2 suggests that O atoms arising from CO bind to reduced centers of titania. ► Preformed Mo particles increase the dispersion of rhodium deposit. ► Extended CO dissociation on Mo-Rh particles stems mainly from reaction with Mo. ► The Mo2C formed is a possible source of enhanced catalytic activity of Mo-Rh clusters.

Research Highlights

► Dissociative adsorption of AsH_3, H_2Se and H_2S on Zn_2TiO_4(010) is studied by DFT.

► Fundamental insight into surface chemistry of trace contaminant removal is provided.

Research highlights

► Cyclopentene interaction with InP(001) is investigated by density functional theory. ► A simple approach for evaluating the surface strain is suggested. ► A linear relation between bond (strain) and adsorption energies is established. ► Charge density associated to the HOMO is more disperse for higher bond energies.

Research Highlights

► Observation of the first polymerization steps between benzene-diboronic acid (BDBA) and hexahydroxy-triphenylene (HHTP) molecules. ► STM observations of different HHTP networks on Ag(111). ► STM observations of the oligomer formation. ► Investigations of the first covalent organic structures. ► Vertical manipulation of HHTP using the STM tip.

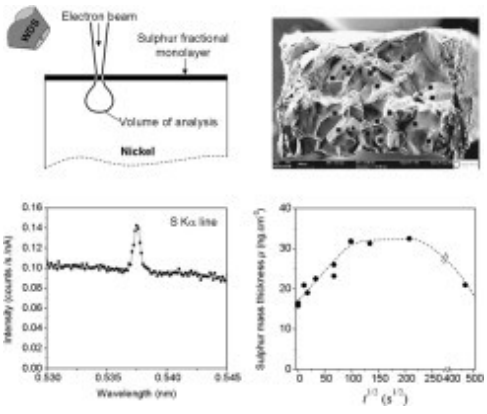
Research highlights

► Step bunching and step rotation are observed in Si/Si(110)-16 × 2 homoepitaxy. ► Step pattern may be tuned by choosing the direction of the electric current. ► Polarity of the applied electrical field has almost no effect the step motion. ► Imperfect matching of the (16 × 2) reconstruction domains induces step bunching.

Research highlights

► Bi atoms are mobile at low coverage on Rh(111) at RT. ► Bi atoms form incommensurate films on Rh(111) except at 0.5 ML. ► At the coverage of 0.5 ML, Bi atoms form a commensurate structure of *c*(2 × 4). ► Bi films transform from twofold structure into sixfold structure above 0.5 ML.

Graphical Abstract



Research Highlights

► WD X-ray Spectroscopy can be used to quantify grain boundary segregation in a SEM. ► The technique can be used on ex-situ fractured samples. ► The precision and limit of detection is a couple of ng.cm^{-2} or percents of a monolayer.