



# GAS-SURFACE NEWS

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## Editors Note

In this issue of Gas-Surface News we have a science report from Axel Groß from the Technische Universität München in which he summarizes his group's research in areas such as first principle calculations of potential energy surfaces for gas-surface interactions and dynamical calculations for dissociative adsorption.

Further good news is that you sent us more than 30 articles submitted or to be published for our list of papers for publication which intends to keep you up to date with the work of your colleagues. It can be found as usual behind our research report. To contact any of the authors you can refer to the GSDList. The articles are followed by detailed information on available research positions, forthcoming meetings and the diary page at the end.

We look forward to hearing from you all and hope you enjoy reading this issue. Please invite any new members of your group to join the mailing list and send me any amendments.

Next Issue - Copy due in June. Please contact me if you wish to contribute in any way.

## GSDList and Web Site

This issue of the Newsletter is also available on the Web site

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You will need the Adobe Acrobat Reader (which is a free download from the Adobe Web site) or a compatible viewer.

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## Research Report

# INTERACTION OF MOLECULES WITH SURFACES FROM FIRST PRINCIPLES

Axel Groß

Physik-Department T30, Technische Universität München, D-85747 Garching, Germany,  
<http://www.ph.tum.de/lehrstuehle/T30g>

### I. OVERVIEW

In September 1998, I moved from the Fritz-Haber-Institut, Berlin, to the Technical University of Munich and started to build up a new research group. While my research in Berlin together with Matthias Scheffler had been mainly focused on the interaction dynamics of hydrogen with metal and semiconductor surfaces (see the research report in the Gas-Surface News No. 22, August 1998), the scope of my research interests has since then broadened. Still the theoretical description of gas-surface dynamics represents an important aspect of my work. In addition, we are performing density functional theory studies of the interaction of molecules with complex structured surfaces. These studies are meant to overcome the materials and structure gap between surface science and, e.g., heterogeneous catalysis. The team doing basically the research work consists of six Ph.D. students at the moment. Applications to join our research group are always welcome, however, the acceptance might also depend on the positions available.

### II. GAS-SURFACE DYNAMICS

The adsorption and desorption dynamics of hydrogen molecules at frozen metal substrates can nowadays be routinely treated within six-dimensional quantum dynamical studies that take all hydrogen degrees of freedom into account [1-3]. We have continued these studies by addressing the dissociation of  $H_2$  on the (2x2) sulfur-covered Pd(100) surface [4-6]. These studies have confirmed the importance of taking the multidimensionality of the adsorption process fully into account. Furthermore, we have addressed the quantum effects in the  $H_2$  dissociation dynamics by comparing classical and quantum dynamics on exactly the same potential energy surfaces [5, 7]. We find that tunneling does not significantly influence the dynamics in the classically allowed energy regime, however, zero-point and quantization effects are often non-negligible.

In a recent five-dimensional quantum study, we have investigated the rotational effects in the adsorption/desorption dynamics of  $H_2$  and  $D_2$  on Pd(100) [8]. In particular, we have focused on the experimentally observed non-monotonous behavior of the rotational alignment in desorption as a function of the rotational quantum number [9,10]. The experimental results are well-reproduced in our calculations (see Fig. 1). We have additionally performed quantum dynamical studies with the hydrogen bond length artificially kept fixed at its gas-phase value. Thus we were able to show that the non-monotonous behavior is caused by the change of the hydrogen bond length upon adsorption and desorption. For low rotational quantum numbers, rotational hindering suppresses adsorption and desorption probabilities. For higher rotational quantum numbers, the change in bond length along the reaction path leads to a decrease in the adiabatic rotational quantum energy which causes an effective energy transfer from rotation to translation. This effect which had already been described

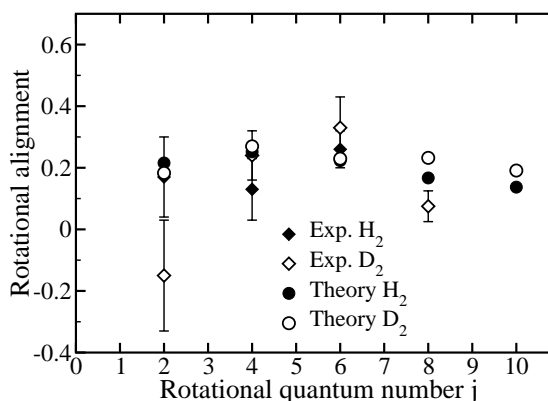


FIG. 1: Comparison of the rotational alignment of  $H_2$  and  $D_2$  molecules desorbing from Pd(100) at a surface temperature  $T_S=700K$  derived from five-dimensional quantum calculations (circles) with the experimental results [9,10] (diamonds). Filled symbols:  $H_2$ , open symbols:  $D_2$  (from [8]).

earlier [11] increases the reaction probabilities and decreases the difference between the reaction probabilities of so-called helicopter and cartwheel molecules leading to a smaller rotational alignment.

If the interaction of molecules heavier than  $H_2$  or  $D_2$  with metal surfaces should be addressed, then the energy transfer to the substrate has to be taken into account in any realistic description. Even more importantly, the energy transfer to the substrate is a necessary ingredient in the modeling of the trapping into molecular adsorption states since no molecule would become permanently trapped without any energy dissipation. Recently, we have been studying the adsorption of  $O_2/Pt(111)$ .  $O_2$  can in fact adsorb both molecularly and dissociatively on  $Pt(111)$ . This system is of great technological relevance since it represents, e.g., one of the fundamental microscopic reaction steps occurring in the car-exhaust catalyst. However, although this system is well-studied, the microscopic reaction steps occurring in the adsorption process had not been identified in detail yet.

The realistic modeling of the adsorption of  $O_2/Pt(111)$  represents a great challenge. First, an accurate potential energy surface is needed that reliably describes both the molecular as well as the dissociative adsorption channels. Secondly, energy transfer to the substrate has to be treated properly by including recoil processes in the first layers of the substrate in order to simulate molecular trapping processes. Since a high-dimensional quantum treatment of  $O_2$  trapping is not possible at the moment, a classical molecular dynamics scheme has to be employed. From our experience with hydrogen systems we conclude that quantum effects should anyway not play a big role in the oxygen adsorption. However, while direct *ab initio* molecular dynamics simulations are too time consuming to calculate a sufficient number of trajectories [12], empirical classical potentials are in general not flexible and accurate enough to describe the bond-making and breaking process on moving substrates.

As a compromise, we have performed tight-binding molecular dynamics (TBMD) simulations [15] of the adsorption of  $O_2/Pt(111)$  using the NRL tight binding (TB) method [16,17] with all TB parameters derived from *ab initio* electronic structure calculations [16, 18]. The calculated sticking probabilities of  $O_2/Pt(111)$  as a function of the kinetic energy for normal incidence are compared to molecular beam experiments [13, 14] in Fig. 2. The calculated sticking probabilities are systematically larger than the

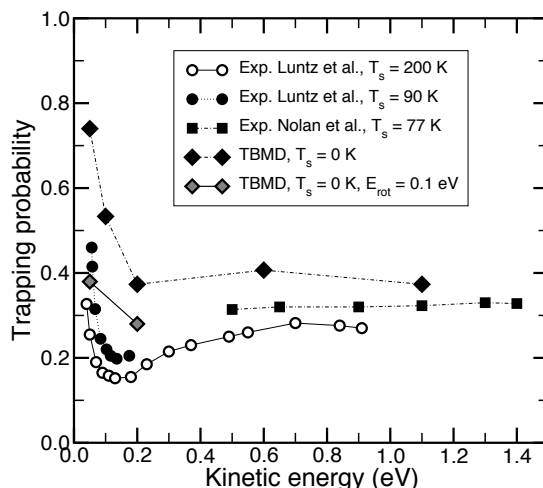


FIG. 2: Trapping probability of  $O_2/Pt(111)$  as a function of the kinetic energy for normal incidence. Results of molecular beam experiments for surface temperatures of 90K and 200K (Luntz et al. [13]) and 77K (Nolan et al. [14]) are compared to tight-binding molecular dynamics simulations for the surface initially at rest (surface temperature  $T_S = 0K$ ).

measured ones which we mainly attribute to the overbinding present in the used DFT-GGA functional [18]. Still, the decrease of the sticking probability at lower kinetic energies and its subsequent saturation are well-reproduced by the TBMD calculations.

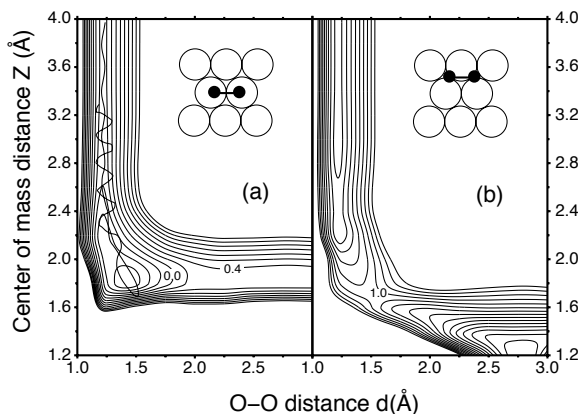
The strong initial decrease of the  $O_2/Pt(111)$  sticking probability has been attributed to the trapping of  $O_2$  into a physisorption state [19] while at higher energies the molecules were assumed to directly access the chemisorbed molecular states [13, 14, 19]. In contrast, our study establishes that the sticking probability over the whole energy range can be understood in terms of trapping into chemisorption states. An analysis of the trajectories reveals that at kinetic energies below 0.2eV all molecules reaching the molecular precursor well get trapped. Thus it is *not* the energy transfer to the substrate *per se* that determines the sticking probability at low kinetic energies but rather the probability to enter the attractive adsorption channels. Although the majority of adsorption pathways is blocked by barriers, at low kinetic energies most of the incoming molecules with unfavorable initial conditions are redirected towards attractive adsorption paths. Thus it is *steering mechanism* as in the system  $H_2/Pd(100)$  that is

responsible for the high sticking probability at low kinetic energies.

This is confirmed by the observed rotational effects on the adsorption dynamics. The steering mechanism is not only strongly suppressed at higher kinetic energies but also by additional rotational hindering. Indeed, we obtain a significant rotational hindering [11], i.e., a strong reduction in the sticking probability, at  $E_i = 0.05$  eV for molecules initially rotating with a rotational energy of  $E_{\text{rot}} = 0.1$  eV, as Fig. 2 shows. A rotational energy of  $E_{\text{rot}} = 0.1$  eV also causes rotational hindering at  $E_i = 0.2$  eV. The assumption of such an initial rotational population of the  $\text{O}_2$  molecules in the molecular beam experiments at this kinetic energy is reasonable. Thus the discrepancy between theory and experiment can partially be accounted for.

At higher energies, the leveling off of the measured sticking probability at higher energy is reproduced by the calculations. To the best of our knowledge, such a behavior has not been obtained before in molecular dynamics simulation which usually yield a monotonously decreasing sticking probability for molecular trapping processes. The underlying mechanism is intimately related to the corrugation and anisotropy of the PES. At such high energies, even molecules with unfavorable initial conditions can get close to the surface. Still there is a negligible probability that in the first collision the high energy particles will transfer enough energy to the surface to remain trapped. However, it is important to note that the impinging molecules also transfer energy into internal molecular degrees of freedom such as rotation and vibration and into lateral motion along the surface. This energy is then not available for a direct escape from the adsorption well. If enough of the initial perpendicular kinetic energy is transferred in the first collision into these other degrees of freedom, the molecule becomes dynamically trapped for a while [20, 21]. While being trapped, the molecule hits the surface several times and transfers successively more and more energy to the substrate until it equilibrates.

Finally, the TBMD simulations have also given an explanation of the surprising experimental result that at surface temperatures below 100 K  $\text{O}_2$  molecules impinging on Pt(111) do not dissociate, even at kinetic energies up to 1.4 eV which are much greater than the dissociation barrier [14, 19]. In fact, no single dissociation event was observed in the molecular dynamics simulations, irrespective of the initial



*Fig. 3: Potential energy surface of the dissociation of  $\text{O}_2/\text{Pt}(111)$  determined by the *ab initio* derived tight-binding Hamiltonian. The coordinates in the figure are the  $\text{O}_2$  center-of-mass distance from the surface  $Z$  and the  $\text{O}-\text{O}$  interatomic distance  $d$ . The configurations of the remaining  $\text{O}_2$  degrees of freedom are illustrated in the insets. The contour spacing is  $0.2$  eV per  $\text{O}_2$  molecule. In (a) a trajectory of an  $\text{O}_2$  molecule with an initial kinetic energy of  $0.6$  eV scattered at  $\text{Pt}(111)$  is also plotted.*

energy. There is a rather simple explanation in terms of the topology of the underlying PES.

Two cuts through the TB potential energy surface of  $\text{O}_2/\text{Pt}(111)$ , so-called elbow plots, are plotted in Fig. 3. They show the PES as a function of the distance  $Z$  of the  $\text{O}_2$  center of mass from the surface and the  $\text{O}-\text{O}$  distance  $d$  while the lateral center of mass degrees of freedom, the molecular orientation and the substrate atoms are kept fixed. While panel (a) corresponds to the superoxo molecular precursor state located above the bridge site which can be accessed along a non-activated path from the gas phase, panel (b) demonstrates the large corrugation of the  $\text{O}_2/\text{Pt}(111)$  PES. Although the molecule is only shifted by about  $1 \text{ \AA}$  in lateral direction compared to panel (a), the nature of the interaction is changed from attraction towards the molecular precursor to strong repulsion with a barrier towards dissociation of almost 1 eV.

Dissociation corresponds to an event in which the molecules enter the exit channel towards the lower right corner of the figures. However, there is a rather narrow curve connecting the entrance and exit channels through the molecular chemisorption states in panel (a). The molecules that enter the chemisorption well become accelerated towards the surface. This makes the molecules so fast that they “do not make it around the corner” into the dissoci-

ation channel. This is illustrated by the projection of a trajectory with  $E_{\text{kin}} = 0.6\text{eV}$  onto the  $Zd$  plane in Fig. 3a. The kinetic energy is much larger than the dissociation barrier. Still the molecule does not dissociate. Due to the acceleration by the attractive potential it hits the repulsive wall of the potential almost straight ahead and is reflected back. This means that direct dissociation of  $\text{O}_2$  is sterically hindered at the Pt(111) surface; dissociative adsorption of  $\text{O}_2/\text{Pt}(111)$  is rather a two-step process. First the molecule is trapped molecularly in the chemisorption well where it equilibrates. At sufficiently high surface temperatures dissociation will then be induced by thermal fluctuations which make the  $\text{O}_2$  molecules enter the dissociation channel.

Concluding the section about the  $\text{O}_2/\text{Pt}(111)$  adsorption, I would like to stress that the presented results can only be obtained and understood if the multidimensionality of the adsorption process is appropriately taken into account. However, in all dynamical simulations presented so far it has been assumed that the electrons stay in their ground state throughout the whole process, i.e., the simulations have been based on the Born-Oppenheimer approximation. Still, at metal surfaces with their continuous spectrum of electronic states at the Fermi energy electron-hole (e-h) pair excitations with arbitrarily small energies are possible. Just recently, experiments determining the so-called chemicurrent [22] have provided some information on the importance of electron-hole pair excitation in adsorption processes. Unfortunately, the incorporation of electronically adiabatic effects in the dynamical simulation of the interaction dynamics of molecules with surfaces is rather difficult. There have been first successful attempts to model the chemicurrent upon adsorption [23], though.

We have been trying to contribute to the understanding of electronically nonadiabatic effects in the interaction of molecules with surfaces. Based on the notion that quantum effects in the dynamics of the nuclei are usually small, we have implemented a mixed quantum-classical surface-hopping scheme based on Tully's fewest switches algorithm. In this approach, the dynamics of the electrons are treated quantum mechanically while the nuclear motion is treated classically [24, 25]. Still, the feedback between quantum and classical degrees of freedom is taken into account self-consistently.

Using this surface hopping scheme, we have addressed the ionization probability in  $\text{I}_2/\text{diamond}$  scattering [24, 25]. The interaction of  $\text{I}_2$  with the dia-

mond surface had been modeled by a potential energy surface that has been adjusted to the few experimental data known for this system. In addition to the molecular center of mass we have included one surface oscillator coordinate, the molecular rotation and vibration. Taking these degrees of freedom into account, we were able to reproduce the observed trend of the ionization probability as a function of the incident kinetic energy of the molecules as well as the measured dissociation probability. According to our model calculations the dependence of the ionization probability on the kinetic energy is not determined by the electronic coupling *per se*, but by the energy transfer to other degrees of freedom during the scattering process. This suppresses the ionization probability because less molecules have sufficient energy to overcome the ionization threshold, in particular at energies close to this threshold. We are currently applying the mixed quantum-classical scheme to the description of the laser-induced desorption of NO.

### III. INTERACTION OF MOLECULES WITH STRUCTURED SURFACES

In recent years, DFT calculations have become an indispensable tool in order to study the interaction of molecules with surfaces [26]. Although there are still limitations in the reliability of DFT results for certain systems, in general DFT studies are very valuable for the elucidation of microscopic details and for establishing chemical trends. Because of more efficient algorithms and the ever-increasing computer power, first-principles electronic structure calculations are no longer limited to the study of simple molecules at low-index surfaces; instead, more and more complex systems can be addressed. For example, the so-called pressure, structure and materials gaps between surface science and heterogeneous catalysis are not only attacked by experimentalists, but also by theorists using electronic structure theory.

In spite of the fact that DFT codes are nowadays routinely applied to surface science problems by many groups, there is still a growing demand for *good* DFT studies. Based on a very fruitful collaboration with G. Kresse and J. Hafner from the University of Vienna, we are employing the VASP code in order to understand the interaction of molecules with structured surfaces such as stepped, precovered or bimetallic surfaces. In a collaboration with the group of Klaus Christmann at the FU-Berlin we have studied the adsorption of hydrogen on Pd(210)

[27,28]. Usually hydrogen adsorbs dissociatively on metal surfaces. On Pd(210), the experimentalists had found the coexistence of adsorbed atomic and molecular hydrogen species but had no clue about the microscopic nature of the adsorption states. Our DFT calculations established that on the clean Pd(210) surface  $H_2$  still dissociates spontaneously. Up to three hydrogen atoms can be adsorbed per (210) surface unit cell corresponding to a coverage of  $\Theta = 3$ . However, for a coverage of  $\Theta = 1$ , the dissociative adsorption of further  $H_2$  molecules becomes activated. Still the attractive interaction of the  $H_2$  molecule with the Pd atoms at the kinked steps of the (210) surface is hardly influenced by the presence of the hydrogen atoms on the surfaces. Thus molecular adsorption wells for the  $H_2$  molecules are created. This means that the molecular adsorption state (see Fig. 4) becomes stabilized by the presence of hydrogen atoms.

As the first part of an ongoing research project about the methanol oxidation on Cu/ZnO catalysts we have studied the dissociative adsorption of  $H_2$  on strained copper surface [29]. This study was motivated by the observation that the methanol oxidation rate could be related to the strain present in small catalytically active Cu crystallites. On all studied Cu surfaces we have found an upshift of the surface  $d$ -band center upon lattice expansion. According to the  $d$ -band model [30] this upshift

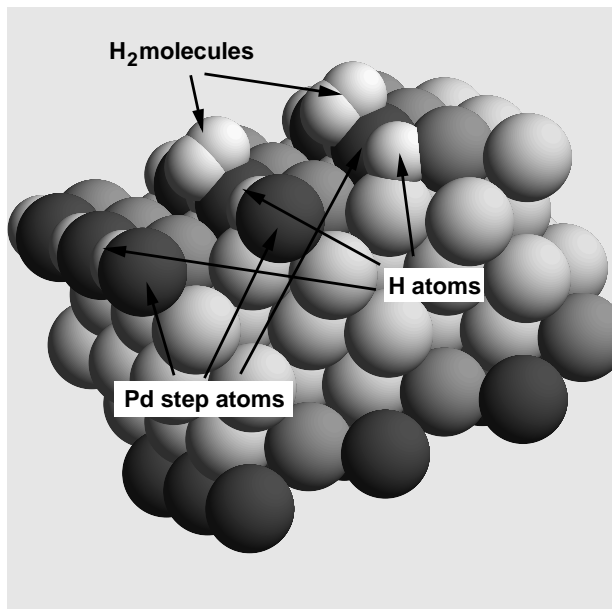


Fig. 4: Side view of the Pd(210) surface with a monolayer H precoverage and the molecular  $H_2$  adsorption state [27].

should be associated with a higher reactivity. Still there is no general trend in the hydrogen adsorption energies at the high-symmetry sites and the dissociation barrier heights as a function of lattice strain. It turns out that the  $d$ -band model is no longer fully appropriate in the case of a strong coupling between adsorbate and substrate; in that case the adsorbate-induced change of the Cu local  $d$ -band density of states has to be taken into account in order to rationalize the results.

We have found similar results for the strain effects in hydrogen adsorption on compressed Pd surfaces [31]. These calculations were part of the investigation of atomic hydrogen and CO adsorption energies on bimetallic  $Pd_n/Au$  overlayer systems with the number  $n$  of overlayers ranging from 1 to 3. Bimetallic surfaces are of strong current interest since they offer the possibility to tailor the surface reactivity by preparing specific surface compositions and structures. The system Pd/Au is of particular interest in the field of electrocatalysis because of its catalytic activities in the oxidation reactions of methanol, formic acid and carbon monoxide. At the same time, it is a prototype system for the study of the reactivity of strained overlayers.

In Fig. 5, the calculated hydrogen and CO adsorption energies as a function of the Pd/Au(111) overlayers are plotted. In addition, the results for a pure Pd(111) substrate with the Pd and the Au lattice constant, respectively, are included in order to disentangle substrate interaction from strain effects for the pseudomorphic overlayers. In general, we find

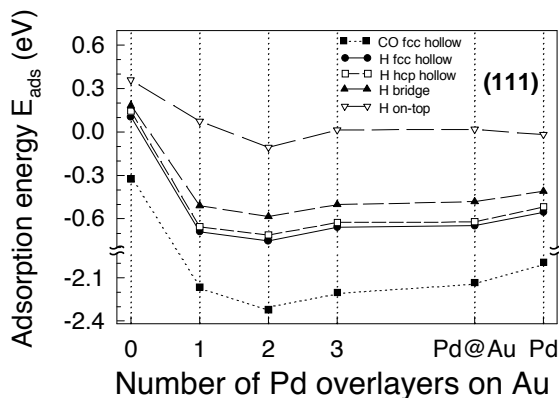


Fig. 5: CO and hydrogen adsorption energies as a function of the number of Pd overlayers on Au for different adsorption sites on the (111) at a coverage of  $\Theta = 0.25$ . The pure Pd substrates with the lateral lattice constant of Au ( $a = 4.18\text{\AA}$ ) and Pd ( $a = 3.96\text{\AA}$ ) are labeled by Pd@Au and Pd, respectively.

that both the lattice expansion of the pseudomorphic Pd films by 5% as well as the interaction of the Pd films with the Au substrate lead to a higher reactivity of the overlayers. This can be rationalized within the *d*-band model. Still, the indirect interaction of the adsorbates with the inert Au substrate on one Pd overlayer reduces the binding energies and leads to a maximum in the binding energies for two Pd overlayers on Au on all adsorption sites that we considered.

On the basis of our findings we thus propose that depositing a reactive metal on an inert metal with a larger lattice constant should in general lead to a higher reactivity of the overlayer since both substrate interaction and strain effects increase the reactivity. Exactly the opposite trend we expect for an overlayer of a less reactive metal deposited on a more reactive metal with a smaller lattice constant, such as, e.g., Pt on Ru. This has in fact been verified in both experiment and theory [32]. We are now extending these studies to the investigation of the reactivity of small Pd clusters supported by Au(111). Further research projects in our group deal with such diverse topics as the adsorbate-induced work function change of tungsten in order to build better cathode discharge lamps or the adsorption of small amino acids on graphite surfaces. However, all projects can be regarded as being part of a joint research effort for the reliable description and analysis of the energetics, kinetics and dynamics of the interaction of molecules with complex surfaces. The knowledge gained so far in theoretical surface science on the route to this ambitious goal has been summarized in a recent text book [33].

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## Papers for Publication

- “Local reactivity of thin Pd overlayers on Au single crystals,” A. Roudgar, A. Groß, J. Electroanal. Chem., submitted
- “An AFM study of the growth kinetics of the self-assembled octadecylsiloxane monolayer on oxidized silicon,” Th. Balgar, R. Bautista, N. Hartmann, E. Hasselbrink, Surf. Sci., in print
- “Incidence angle dependence of scattering and dissociation of O<sub>2</sub> on Al(111): Possible weakly bound molecular precursors,” O. Weiße, C. Wesenberg, M. Binetti, E. Hasselbrink, C. Corriol, G. R. Darling, St. Holloway, J. Chem. Phys., in print
- “The role of non-adiabatic pathways and molecular rotations in the oxygen abstraction reaction on the Al(111) surface,” M. Binetti, O. Weiße, E. Hasselbrink, G. Katz, R. Kosloff, Y. Zeiri, Chem. Phys. Lett., accepted
- “Catalytic and non-catalytic CO oxidation on Au/TiO<sub>2</sub> catalysts,” J. Soares, P. Morrall, A. Crossley, P. Harris, M. Bowker, J. Cat., submitted
- “NO<sub>x</sub> storage in model Pt/NSR catalysts: Fabrication and reactivity of BaO nanoparticles on Pt(111),” P. Stone, M. Ishii, M. Bowker, Surf. Sci., submitted
- “Formic acid adsorption and oxidation on Cu(110),” T. Youngs, S. Haq, M. Bowker, Surf. Sci., submitted
- “Modification of catalysis and surface reactions by surface carbon,” M. Bowker, C. Morgan, J. Couves, Appl. Cat., submitted
- “Acetic acid adsorption and decomposition on Pd(110),” M. Bowker, C. Morgan, J. Couves, Surf. Sci., submitted
- “NO<sub>x</sub> storage and reduction on Pt/BaO catalysts,” D. James, E. Fourre, M. Ishii, M. Bowker, Appl. Cat., submitted
- “The mechanism of Si etching in fluoride solutions,” K. W. Kolasinski, Phys. Chem. Chem. Phys., accepted
- “Low energy vibrational dynamics of Xe on copper,” Ch. Boas, M. Kunat, U. Burghaus, B. Gumhalter, Ch. Wöll, Phys. Rev. B, submitted
- “Adsorption of CO on rutile (1x1)-TiO<sub>2</sub>(110): A molecular beam study,” M. Kunat, U. Burghaus, Surf. Sci., submitted
- “Kinetic Monte Carlo simulation of adsorption probabilities: The auto-catalytic adsorption phenomenon,” J. Stephan, U. Burghaus, AVS-Denver, J. Vac. Sci. Tech., in press
- “Stabilization of polar ZnO-surfaces: Validating microscopic models by using CO as a probe molecule,” V. Staemmler, K. Fink, B. Meyer, D. Marx, M. Kunat, S. Gil Girol, U. Burghaus, Ch. Wöll, Phys. Rev. Lett., in press
- “State resolved inelastic scattering of N<sub>2</sub> from Ru(0001),” H. Mortensen, E. Jensen, L. Diekhöner, A. Baurichter, A. C. Luntz, V. V. Petrunin, accepted
- “Linear vs. nonlinear coupling effects in single- and multi-phonon atom-surface scattering,” A. Sibener, B. Gumhalter, Phys. Rev. Lett., accepted
- “Diffraction of He atoms from Xe monolayer adsorbed on the graphite(0001) revisited: The importance of multiple scattering processes,” A. Sibener, B. Gumhalter, Surf. Sci., accepted
- “Microcalorimetric, infrared spectroscopy and DFT studies of Co adsorption on Rh and Rh-Te catalysts,” R. He, H. Kusaka, M. Mavrikakis, J. A. Dumesic, J. Catal., in press
- “DFT studies for cleavage of C-C and C-O bonds in surface species derived from ethanol on Pt(111),” R. Alcalá, M. Mavrikakis, J. A. Dumesic, J. Catal., in press
- “Atomic scale evidence for an enhanced catalytic reactivity of stretched surfaces,” J. Wintterlin, T. Zambelli, J. Trost, J. Greeley, M. Mavrikakis, Angewandte Chemie International Edition, in press
- “Angular distribution of H<sub>2</sub> molecules scattered from the Pd(111) surface,” C. Díaz, H. F. Busnengo, F. Martín, A. Salin, J. Chem. Phys., accepted
- “Role of dynamic trapping in H<sub>2</sub> dissociation and reflection on Pd surfaces,” M. A. Di Césare, H. F. Busnengo, W. Dong, A. Salin, J. Chem. Phys., submitted



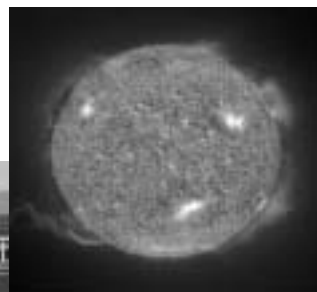
- “Active role of oxide support during CO oxidation at Au/MgO,” L. M. Molina, B. Hammer, submitted
- “Thermal chemistry of acetylene and ethylene on Ni(100) studied by in-situ x-ray photoelectron spectroscopy,” R. Neubauer, C. M. Whelan, R. Denecke, H.-P. Steinrück, *J. Chem. Phys.*, submitted
- “Vibrations of a chain of Xe atoms in a groove in a carbon nanotube bundle,” M. T. Cvitas, A. Siber, *Phys. Rev. B*, accepted
- “Quantum virial expansion approach to thermodynamics of  $^4\text{He}$  adsorbates in carbon nanotube materials: Interacting Bose gas in one dimension,” A. Siber, *Phys. Rev. B*, accepted
- “Surface functionalization of Ni(111) with acrylate monolayers,” B. S. Yeo, Z. H. Chen, W. S. Sim, *Langmuir*, in press
- “Steric effect in electron-molecule interaction,” Y. Lilach, M. Asscher, submitted
- “Patterning metallic thin films at the nanometer scale by laser desorption of weakly bound buffer layers on surfaces,” G. Kerner, M. Asscher, submitted
- “Adsorption of  $\text{NH}_3$  on oxygen-pre-treated Ni(111),” E. Laksono, A. Galtayries, C. Argile, P. Marcus, *Surf. Sci.*, in press
- “Molecular dynamics simulation of palladium cluster growth on flat and rough graphite surfaces,” P. Brault, G. Moebs, *Phys. Rev. E*, submitted
- “Critical behavior in an atomistic model for a bistable surface reaction: CO-oxidation with rapid CO diffusion,” N. Pavlenko, R. Imbihl, J. W. Evans, D.-J. Liu, *Phys. Rev. E*, submitted
- “Crossover between mean-field and ising critical behavior in a lattice-gas reaction-diffusion model,” D.-J. Liu, N. Pavlenko, J. W. Evans, *J. Stat. Phys.*, submitted, submitted
- “Geometry-based simulation of submonolayer film growth,” M. Li, M. C. Bartelt, J. W. Evans, *Phys. Rev. Lett.*, submitted

## International Summer School “Towards a Hydrogen-based Society”



August 9-15, 2003

Krogerup Højskole  
Humlebæk, Denmark



**Interdisciplinary Research Center for Catalysis (ICAT),  
Technical University of Denmark, Lyngby, Denmark**

## INTERNATIONAL SUMMER SCHOOL “TOWARDS A HYDROGEN-BASED SOCIETY”

The international summer school “Towards a Hydrogen-Based Society” is directed primarily towards young scientists, e.g. PhD students throughout the world who have an interest in technologies connected to the vision of the “Hydrogen Society”. The program consists of a series of lectures given by well know and leading international experts within the different areas of the hydrogen technology. Plenty of time will be reserved for discussions in smaller groups and in plenum of the different results and views presented by the experts. It is also envisioned that the participants each bring materials for presenting a poster at the summer school in order to stimulate interaction and discussions in between the participants on their own projects, making contacts that may last and inspire beyond the summer school. The language of the summer school is English.

**The summer school is sponsored by:**

- the Danish Research Agencies through the Center of Excellence “Towards a Hydrogen-Based Society”
- INANO graduate school, INANO is the Interdisciplinary Nanoscience Center at University of Aarhus (<http://www.inano.dk/>)
- Copenhagen Nanoscience Academy

**Program:**

The main themes for the international summer school “Towards a Hydrogen-Based Society” are hydrogen production, hydrogen storage, and hydrogen conversion. Also subjects such as the economical and environmental aspects of the hydrogen vision will be treated. The program will include invited lectures from leading international experts, group work for the participating students, and poster sessions where all students should present a poster. Furthermore, excursions to the nearby Modern Art Museum “Louisiana” and Copenhagen City are planned.

**General information:**

The international summer school “Towards a Hydrogen-based Society” will take place on August 9-15, 2003, at Krogerup Højskole in Humlebæk, Denmark. It starts on August 9 at 17:00 (arrival from 15:00) and it ends on August 15 at 15:00.

Humlebæk is located in North Zealand, approximately 40 km from the Copenhagen Airport (Kastrup) and 30 km from Copenhagen Central Station. Trains depart every 20-30 minutes from both the airport and the station directly to Humlebæk.

The registration fee is DKr 3.000. The fee covers participation in the summer school, accommodation in double rooms at Krogerup Højskole for the nights of August 9-14, all meals and refreshments (coffee) during the summer school, and the excursions. We are not able to give any support towards travel expenses or to waiver the registration fee for the participants.

**FUNDAMENTAL ASPECTS AND PRACTICAL APPLICATIONS  
OF SURFACE DIFFUSION**

**Institute of Physics, Academy of Sciences of the Czech Republic**

**September 14 - 17, 2003 Trest, Czech Republic**

**Major Topics include:**

Diffusion and Phase Transitions  
Diffusion in Biological and Soft-Matter Systems  
Acceleration Methods in Diffusion  
Diffusion and Growth  
Diffusion under Non-Equilibrium condition  
Novel Approach to Diffusion  
Round table discussion on: Current State of Surface Diffusion - What's in the Future?

**Format of the Workshop:**

Invited speakers from leading groups will present their results, and there will also be contributed oral and poster contributions as well as specific topical discussions to permit an active participation of all participants.

**Program Committee:**

Tapio Ala-Nissila, Laboratory of Physics, Helsinki University of Technology, Helsinki, Finland  
Zdenek Chvoj, Institute of Physics AV CR, Prague, Czech Republic  
Peter J. Feibelman, Sandia National Laboratories, Albuquerque, New Mexico, USA  
Riccardo Ferrando, University of Genova, Genova, Italy  
Joost W. M. Frenken, Leiden University, Leiden, The Netherlands  
Michael C. Tringides, Ames Laboratory, Iowa State University, Ames, Iowa, USA  
See Chen Ying, Brown University, Providence, Rhode Island, USA

**Deadline Instructions:**

Abstract submission and preliminary registration: April 30, 2003  
Notification of acceptance: May 30, 2003  
Registration and registration payment: June 30, 2003

**Abstract Submission:**

Authors of contributed presentations should send a one page abstract to Prof. Tapio Ala-Nissil or Zdenek Chvoj by email until April 30, 2003. The program committee will provide information on acceptance and scheduling of the presentations by May 30, 2003.

For further information and pre-registration see the Workshop official website. Our meeting is Satellite Workshop (CZ Trest) to ECOSS22, held in Prague: <http://ecoss.fzu.cz/> (and click to satellite workshop)

RNDr., DrSc.  
Institute of Physics AV CR  
Cukrovarnicka 10  
162 53 PRAHA 6  
CZECH REPUBLIC

Fax: +420 233 343 184  
e-mail: [chvoj@fzu.cz](mailto:chvoj@fzu.cz)  
tel.: +420 220 318 530  
Helsinki University of Technology  
Laboratory of Physics  
P.O.Box 1100  
FIN-02015 HUT  
ESPOO, FINLAND

## INTERNATIONAL MEETING ON APPLIED PHYSICS (APHYS-2003)

October 14<sup>th</sup>-18<sup>th</sup> 2003 in Badajoz (Spain)

All the information regarding this interdisciplinary conference can be found at the conference website [www.formatex.org/aphys2003/aphys2003.htm](http://www.formatex.org/aphys2003/aphys2003.htm).

The Call for Abstracts is open.

Some of the topics to be covered will be:

- Surfaces, Interfaces and Colloids
- Imaging Techniques, Microscopy
- Nano-Sciences and Technologies
- Biophysics and Biophysical Chemistry
- Materials Science & Engineering, Applied Solid State Physics/Chemistry
- Advanced and Functional Materials
- Biomedical Engineering and Biomaterials
- Biological & Medical Physics
- Computational Physics
- Radiation Physics, Applied Nuclear Physics/Chemistry, Radiation Protection

In addition to the regular scientific program, several international workshops will be held as pre-conference events. The following workshops are presently confirmed:

1. Workshop on Modern Applied Microscopy in Molecular and Cell Biophysics Research
2. International Interdisciplinary Workshop on Bioengineered Non-Crystalline Solids
3. Workshop on Interfaces in Colloidal and Particulate Systems
4. International Workshop on Radiation Protection and Dosimetry

The conference will be specifically interested in receiving reports on interdisciplinary researches relating physics with other sciences such as biology, chemistry, information technology, medicine, etc or relating different physics areas. In other words, we are specially (but not exclusively) interested in reports applying the techniques, the training, and the culture of physics to research areas usually associated with other scientific and engineering disciplines.

APHYS-2003 will also serve as a platform to search for partners for transnational collaboration projects, especially for the EU Sixth Framework Program (NETworks of Excellence and Integrated Projects). "Projects Presentations" and "Call for Partners" presentations proposals are therefore encouraged and welcomed. If you are interested in taking part in this conference feature, please send us the corresponding form available at the website.

In addition to the "traditional" oral contribution and posters presentation, a virtual participation modality has been established for those researchers unable to attend it in person. A limited number of works can be presented in this way. Please refer to the conference website for details.

If you are interested in taking part in APHYS-2003, please send us your PRE-REGISTRATION FORM (at the main website of the conference) as soon as possible. The pre-registration form is also available through the direct URL <http://www.formatex.org/aphys2003/preregistration.htm>.

Deadline for abstracts submission is April 30<sup>th</sup> 2003 (for oral presentations proposals; for posters additional time will be provided) although we highly recommend you to submit your abstract as soon as possible to avoid saturation during the days before the deadline.

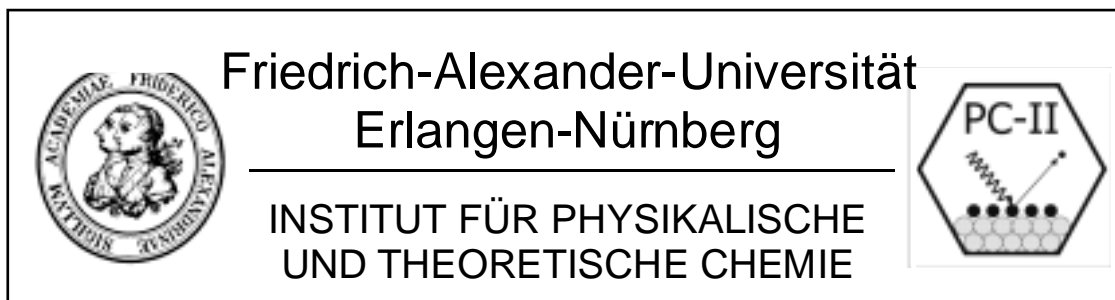
### Proceedings:

Accepted and presented papers will be reviewed for publication in special issues of several international journals such as Journal of Microscopy, Journal of Non-Crystalline Solids, Applied Surface Science, Surfaces and Colloids A, Powder Technology (to be confirmed), Microelectronics Journal, Physica Scripta, Radiation Protection Dosimetry and Applied Physics A, Materials Science & Processing (to be confirmed) and Bio-Medical Materials & Engineering. Also a book "Advances in Applied Physics" will be published by an international publisher (Kluwer or American Institute of Physics), with those papers accepted for presentation but not suita-

ble for the journal issues. For up-to-date information on publications participating at the conference as publishers, please visit regularly the conference website (proceedings sections).

For any question or suggestion, please do not hesitate to contact us at [secretariat@formatex.org](mailto:secretariat@formatex.org), or visit [www.formatex.org/aphys2003/aphys2003.htm](http://www.formatex.org/aphys2003/aphys2003.htm) (Bookmark the page!!). We would also appreciate if you could disseminate this call for papers through your department or institution. We hope to meet you at this exciting and interdisciplinary meeting!

J. A. Mesa Gonzalez  
APHYS-2003 Secretariat  
Email: [secretariat@formatex.org](mailto:secretariat@formatex.org)



### Postdoctoral-Position

A postdoctoral position (Wiss. Assistent, C1) is available at the Institute of Physical Chemistry in the group of Prof. Hans-Peter Steinrück. The research activities focus on surface and interface science. Besides studies of single crystal and polycrystalline surfaces, we are particularly interested in designing new materials with novel electronic, geometric and chemical properties. Special attention is paid on tailoring of these properties on the nanometer scale. The materials include ultrathin metal and oxide layers on metal substrates as well as molecular layers on metals.

We apply a variety of experimental methods, including high resolution X-ray photoelectron spectroscopy (XPS) and angle-resolved UV photoelectron spectroscopy (ARUPS), partly using synchrotron radiation, as well as low energy electron diffraction (LEED), molecular beam techniques and scanning tunneling microscopy (STM). The candidate is expected to participate in running research programs and to establish new activities within the research group.

Candidates with a PhD in physics or physical chemistry, who are interested in joining an interdisciplinary research team should contact:

Prof. Dr. Hans-Peter Steinrück  
Institut für Physikalische und Theoretische Chemie  
Universität Erlangen-Nürnberg  
Egerlandstraße 3  
D-91058 Erlangen  
Germany  
Tel.: +49 (0)9131 85-27343  
Email: [steinrueck@chemie.uni-erlangen.de](mailto:steinrueck@chemie.uni-erlangen.de)  
<http://www.chemie.uni-erlangen.de/pc2/>

**University of Reading**  
**Postdoctoral Fellowship in Surface Science**

This position is in the Centre for Surface Science and at Cardiff University, Wales and occurs just after the move of our group there in August this year. It will concern the fabrication of metal nanoparticles on the surface of single crystal bulk oxides (e.g.  $\text{Fe}_2\text{O}_3$ ,  $\text{TiO}_2$ ), and the characterisation of these materials by variable temperature STM, by XPS, by TPD and by molecular beam measurements of reactivity.

Experience in surface science methodology is essential for the postdoctoral position, though further training will be given. For more details of the work of the group please see our web page. For further information, or to apply, contact:

Professor Mike Bowker  
Dept. Chemistry  
University of Reading  
Whiteknights Park  
Reading RG6 6AD  
England  
Tel.: +44 (0)118 931-6602  
email: [m.bowker@rdg.ac.uk](mailto:m.bowker@rdg.ac.uk)  
<http://www.chem.rdg.ac.uk/dept/catrg/catrg.html>

The closing date for applications is May 1<sup>st</sup>.



**School of Chemistry  
University of St. Andrews**

**Postdoctoral Research Assistant**

Within the rapidly developing and well-equipped research field of Surface Science, the School of Chemistry at St. Andrews (<http://chemistry.st-and.ac.uk/>) is seeking to fill an EU supported, postdoctoral research assistant post with immediate effect. The post, tenable for two years in the first instance, is associated with a Research Training Network on "*The exploitation of molecular motion of molecular architectures*". Other partners in the network are based in the UK, France, Italy and The Netherlands. The successful candidate will be expected to spend short periods working in partners' laboratories, to attend network meetings and international conferences.

Suitable candidates will hold a doctorate in an appropriate discipline; Chemistry, Physics or Material Science with a proven research background and relevant practical experience in UHV technologies, scanning probe microscopies or other techniques of surface characterisation.

Applications should be made to Professor N. V. Richardson ([NVR@st-andrews.ac.uk](mailto:NVR@st-andrews.ac.uk)).

Applicants should send a CV and arrange for two academic references to be forwarded by the closing date of 10<sup>th</sup> April 2003.

Professor Neville V. Richardson  
School of Chemistry, North Haugh  
University of St. Andrews  
St. Andrews, Fife KY169ST  
Scotland  
Tel.: +44 1334 462395  
Fax: +44 1334 467285

**Laboratoire de Physique des Interfaces et Couches Minces (LPICM)  
Ecole Polytechnique  
91 128 Palaiseau  
[http://www.ecoledoctorale.polytechnique.fr/WEBAnglais/Monge\\_eng.html](http://www.ecoledoctorale.polytechnique.fr/WEBAnglais/Monge_eng.html)\***

**Proposal for a PhD subject**

PhD director : Marc CHATELET, directeur de recherche au CNRS  
[Chatelet@leonardo.polytechnique.fr](mailto:Chatelet@leonardo.polytechnique.fr)

**Title:**

Interaction of mixed metal-carbon compounds clusters with a structured surface: experimental study of the growth of singlewall carbon nanotubes (SWCNT); chirality control

It has been shown that during the impact of large van der Waals clusters on hard surfaces the supersonic clusters undergo an ultrafast heating and a large pressure increase and they deliver a large transfer of momentum. The nano-shock conditions and impulsive nature of interactions in the newly formed compressed nonequilibrium environment open avenues for studying chemical reactivity and dynamics catalyzed via cluster impact. That would be during such impact process between clusters containing both the metal catalyst and the carbon compounds and a structured substrate we will study the growing reaction of the carbon nanotubes. Such studies would bring a better understanding of the elementary process of the SWCNT and then allow a chirality control.

The large mixed clusters will be prepared by the pick up technics of transition metal by a supersonic molecular beam of rare gas. In a first step, we will study the pick up of metal atoms issued from the metal vapor (cobalt, iron or nickel), by rare gas clusters passing through the buffer metal gas. We will investigate then the deposit of the catalyst on a substrate by collision of this mixed cluster beam and the substrate. The deposited metal atoms will migrate due to their mobility on the surface in order to form cluster islands. We will study how the preparation parameters influence the catalyst properties of those islands.

In a second step, we will investigate the growth of the SWCNT on these precursor cluster islands. We will use carbonated gas as CO, CH<sub>4</sub> or C<sub>2</sub>H<sub>2</sub> in the cluster beam. The control of the nanotube chirality will depend on the properties and the selection of the cluster islands.

In parallel, we will try to get some mixed clusters containing both the catalyst metal and the carbon compounds in order to initiate the growth reaction directly inside the cluster during the impact with the surface.

In order to make this experimental work, the PhD student will work with a supersonic molecular beam delivering clusters, and with ultra vacuum equipment including several diagnostics as mass spectroscopy, different energy electron scatterings, tunneling microscopy and laser spectroscopy.

Information about the PhD fellowship can be found in :

[http://www.ecoledoctorale.polytechnique.fr/WEBAnglais/Monge\\_eng.html](http://www.ecoledoctorale.polytechnique.fr/WEBAnglais/Monge_eng.html)

**Postdoctoral Research Associates in Surface Science  
Research Group of Charles T. Campbell  
University of Washington  
Seattle, WA**

The research group of Charles Campbell at the University of Washington in Seattle, WA, USA is seeking two postdoctoral research associates in different areas of surface science. The starting salary is \$36,500. A PhD degree in Chemistry, Physics or Chemical Engineering is required. Experience with experimental techniques of surface science is strongly preferred.

(See <http://www.cpac.washington.edu/~campbell/> for details of group's activities.) Individuals are sought to contribute to our research programs in one or two of the following areas:

1. Metal / polymer and metal / organic interfaces: These form an important part of many polymer-based and organic-based opto-electronic devices. We investigate the electronic properties that control the electron and hole transport / injection properties of these interfaces, and measure their interfacial binding energetics by adsorption calorimetry.
2. Self-assembly processes in nanofabrication: We have a novel method of producing ordered arrays of quantum dots on clean surfaces under ultrahigh vacuum, and use these to study self assembly processes that might be used to add hierarchical structures and interconnects to these.
3. Metal nanoparticles on oxide supports: These are important in catalysis, and we study their chemical, electronic and catalytic properties, and correlate these with their energetics.

Apply to:

Dr. Charles T. Campbell  
Professor and Co-Director of the Center for Nanotechnology  
University of Washington  
Department of Chemistry, Box 351700  
On express mail (not regular mail), add: 36 Bagley Hall  
Seattle, WA 98195-1700  
USA  
email: [campbell@chem.washington.edu](mailto:campbell@chem.washington.edu)  
Web: <http://www.cpac.washington.edu/~campbell/>  
phone: +1 (206)616-6085  
fax: +1 (206) 616-6250

**31<sup>st</sup> March - 4<sup>th</sup> April 2003**

**The Third San Luis Symposium on Surfaces, Interfaces and Catalysis, Mérida, Venezuela**

More information can be found at the web site: <http://www.chem.ucr.edu/Zaera/SanLuisIII/>, organizer is Francisco Zaera, Department of Chemistry, University of California, Riverside, CA 92521, USA, phone: +01 909 787-5498, fax: +01 909 787-3962, e-mail: [francisco.zaera@ucs.edu](mailto:francisco.zaera@ucs.edu), web site: [www.chem.ucr.edu/Zaera/lab.html](http://www.chem.ucr.edu/Zaera/lab.html)

**9<sup>th</sup>-15<sup>th</sup> August 2003**

**International Summer School "Towards a Hydrogen-Based Society", Krogerup Højskole, Humlebæk, Denmark**

The registration form can be downloaded from the summer school home page <http://www.fysik.dtu.dk/~helle/summer2003.html> and should be faxed to Helle Wellejus at fax number +45 4593 2399 or e-mailed to [helle@fysik.dtu.dk](mailto:helle@fysik.dtu.dk) before 1<sup>st</sup> June 2003.

**10<sup>th</sup>-15<sup>th</sup> August 2003**

**Gordon Research Conference on Dynamics at Surfaces, Andover, USA**

Chair: Stephen Holloway, Liverpool. Conference application information can be obtained from the [GRC website](#) or by email: [grc@grcmail.grc.uri.edu](mailto:grc@grcmail.grc.uri.edu).

**14<sup>th</sup>-17<sup>th</sup> September 2003**

**Fundamental Aspects and Practical Application of Surface Diffusion, Trest, Czech Republic**

For further information and pre-registration see the workshop official website: <http://ecoss.fzu.cz/>. You can also send a fax to +420 233 343 184 or e-mail to [chvoj@fzu.cz](mailto:chvoj@fzu.cz).

**14<sup>th</sup>-18<sup>th</sup> October 2003**

**International Meeting on Applied Physics (APHYS-2003), Badajoz, Spain**

All the information regarding the conference can be found at the conference website <http://www.formatex.org/aphys2003/aphys2003.htm>. E-mails can be sent to [secretariat@formatex.org](mailto:secretariat@formatex.org).

**11<sup>th</sup>-15<sup>th</sup> January 2004**

**Workshop: Nonadiabatic Processes at the Gas-Surface Interface, Ein-Gedi, Israel**

All the information regarding the conference can be obtained from [eva@fh.huji.ac.il](mailto:eva@fh.huji.ac.il).