

SCHLOSS RINGBERG

October 29 to November 1, 2017

Symposium on Dynamics at Surfaces



Sunday, October 29	
16:00	Arrival and registration
18:30	Dinner
19:30	Informal Discussions
21:00	Poster Session I
Monday, October 30	
08:00-9:00	Breakfast
9:00	Alec Wodtke <i>Welcoming Remarks and Overview</i>
<i>Session Chair: Dr. Sascha Kandratsenka</i>	
9:30	Altschäffel, Jan: <i>Minimum energy pathways for the dissociation diatomics on metal(111) surfaces</i>
10:00	Jiang, Hongyan <i>Threshold energy and dynamics of C-H[D] bond formation on epitaxial graphene at zero surface coverage</i>
10:30	Coffee Break
11:00	Kammler, Marvin: <i>Hydrogen atom scattering from a free-standing graphene surface</i>
11:30	Sven Meyer <i>Scattering NO from Pt(111) and graphene/Pt(111)</i>
12:00	Artur Meling <i>Scattering of NO from thin film VO₂ surface</i>
12:30	Lunch Break
<i>Session Chair: Dr. Tim Schäfer</i>	
14:00	James Johns (invited) tba
15:00	free time
18:30	Dinner
20:00-	Poster Session II
Tuesday, October 31	
8:00-9:00	Breakfast
<i>Session Chair: Dr. Kai Golibrzuch</i>	
9:00	Thomas Miller (invited): <i>New theoretical methods for chemical dynamics at surfaces</i>

10:00	Chen, Li: <i>Vibrational dynamics of molecules at interfaces studied with laser-induced infrared fluorescence spectroscopy</i>
10:30	Coffee Break
11:00	Lau, Jascha <i>Vibrational Energy Pooling in a CO/NaCl(100) Monolayer: Kinetic Monte Carlo Simulations</i>
11:30	Kumar, Sumit <i>Surprisingly long-lived vibrational lifetime of CO on Au(111): A time resolved sum frequency generation study</i>
12:00	Wagner, Roman <i>Scattering highly vibrationally excited CO from an Au(111) surface</i>
12:30	Lunch Break
<i>Session Chair: Dr. Tim Schäfer</i>	
14:00	Pan, Xiulian <i>Challenges and opportunities in C1 chemistry</i>
15:00	Free time
18:30	Dinner
21:00-	Poster Session III
Wednesday, November 1	
8:00-9:00	Breakfast
<i>Session Chair: Prof. Dirk Schwarzer</i>	
9:00	Borodin, Dima <i>Velocity-resolved kinetics using ion imaging – CO oxidation and trapping at atomically stepped surfaces</i>
9:30	Papendorf, Kim <i>Post-permeation associative desorption of hydrogen from an Ag(111) surface</i>
10:00	Coffee Break
10:45	Park, Barratt <i>Investigating mode specificity of nonadiabatic behavior at surfaces</i>
11:30	Prof. Alec Wodtke: <i>Closing Remarks</i>
12:00	Getting Lunch Packages and Departure

ABSTRACTS

Ultrafast photo-induced electron transfer in self-assembled donor-acceptor coordination cages and Prussian Blue Analogues.

Jennifer Ahrens

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This work focuses on the investigation of photophysical properties of different supramolecular metal complexes, which were characterized by femtosecond pump-probe spectroscopy. In this work two different metal complexes were analysed. On the one hand, Pd(II) complexed donor-acceptor double cages based on phenothiazine (D) and anthraquinone (A) ligands were examined with regard to a photoinduced charge separation and thus their potential use for photovoltaic applications. On the other hand, Prussian Blue Analogues were considered which are known for their switchable spin and redox states. Particularly in relation to information processing at molecular level they offer a potential application field as nanoscale electronic components. In this work the focus of investigation lies on dinuclear and tetranuclear Fe/Co Prussian Blue Analogues and their ability for CTIST (charge transfer induced spin transition).

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Minimum energy pathways for the dissociation of diatomics on metal(111) surfaces

Jan Altschäffel, Alexander Kandratsenka and Alec M. Wodtke

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Dissociation of molecules on metal surfaces is an elementary step in heterogeneous catalysis and so plays an important role in many industrial applications. To understand the energetics of dissociation processes we carried out the minimum energy path DFT calculations on the GGA-level with the FHI-aims code [1]. We were particularly interested in the geometry of the transition state, so we used the string method to evaluate the minimum energy pathway (MEP) and then by means of the climbing image method we determine the transition state more accurately [2]. We focus on the systems, which were experimentally studied in our group, such as HCl/Au(111), NO/Au(111) and NO/Ag(111) [3],[4].

MEP calculations related to the CO oxidation on Pt(111) for different CO coverages are presented, too.

[1]: V. Blum et al., *Comp. Phys. Comm.*, **180**, p. 2175–2196, **2009**.

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[4]: B. C. Krüger et al., *J. Phys. Chem. Lett.*, **7**, p. 441–446, **2016**.

Velocity-Resolved Kinetics using Ion Imaging - CO oxidation at Atomically Flat and Stepped Pt and Pd Surfaces

D. Borodin, J. Neugeboren, M. Schwarzer, H. W. Hahn, D. J. Harding, D. Schwarzer, A. Kandratsenka, D. J. Auerbach, C. T. Campbell, A. M. Wodtke, T. N. Kitsopoulos.

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The present work offers a detailed study of the reaction dynamics and kinetics of the CO oxidation on Pt(111), Pt(332) and Pd(111) by means of molecular beams, spatial ion imaging and velocity-resolved kinetics^[1].

Experiments at platinum and palladium surfaces shows a bimodality in the kinetic energy distribution of the CO₂ product. The slow channel has kinetic energies close to those expected from molecules in equilibrium with the surface temperature, while the fast channel has a much higher kinetic energy release. The thermal component is the dominant pathway for the formation of CO₂ at Pt(332), while a larger fraction of the hyperthermal CO₂ component contributes to the overall flux at Pt(111) and Pd(111). We could assign the thermal CO₂ component to be formed at atomic steps and the hyperthermal component to be formed at terraces.

We have developed a kinetic mechanism which includes three elementary CO₂ forming reactions at steps and terraces^[2]. From our new approach to measure reaction kinetics at surfaces we can derive product flux vs. reaction time profiles. In combination with numerical modeling we are able to derive the elementary rate constants for three CO₂ forming reactions at the platinum and palladium surfaces. In contrast to previous studies, we do not find evidence for a coverage dependent activation energy as proposed in previous studies. We claim that these effects result from the fact that previous works were not sensitive for elementary step reactions of CO₂ formation.

- [1] D. J. Harding, J. Neugeboren, H. Hahn, D. J. Auerbach, T. N. Kitsopoulos, A. M. Wodtke, *J. Chem. Phys.* **2017**, *147*, 013939.
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Femtosecond pump-probe-spectroscopy in condensed xenon- elucidation of the electronic structure and relaxation dynamics in search of solvated electrons

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Solvated electrons are well known for over two decades^[1] from deep blue solutions produced by dissolving alkali metals in ammonia^[2]. The color originates from their broad intense absorption band in the visible spectral region^[3]. Although a strong dependence of the position of the band on the solvent is apparent^[3] and polar liquids like water and ammonia were investigated thoroughly^[4], little is known about the exact mechanics and dynamics of their stabilization in nonpolar media.

In order to find solvated electrons and possibly understand their formation and relaxation or decay dynamics in quite nonpolar^{[5],[6]}, however highly polarizable^[7] supercritical xenon, femtosecond multiphoton-UV/VIS-pump-near-IR-probe-spectroscopy was used. Prior to this, analysis of the electronic structure of xenon in gaseous, solid and liquid phase was conducted to find appropriate wavelengths for pump (creation) and probe (excitation) beam.

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Vibrational dynamics of molecules at interfaces studied with laser-induced infrared fluorescence spectroscopy

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We perform frequency- and time-resolved laser-induced infrared fluorescence spectroscopy (LIIF) measurements to study dynamics of molecular vibrational energy flow at solid interfaces. Using an ultra-sensitive infrared emission spectrometer equipped with a superconducting nanowire single-photon detector (SNSPD), we are able to detect molecular emission in a broad spectrum range (2-7 μm) of mid-infrared with *sub-monolayer sensitivity* and *sub-nanosecond* time resolution.

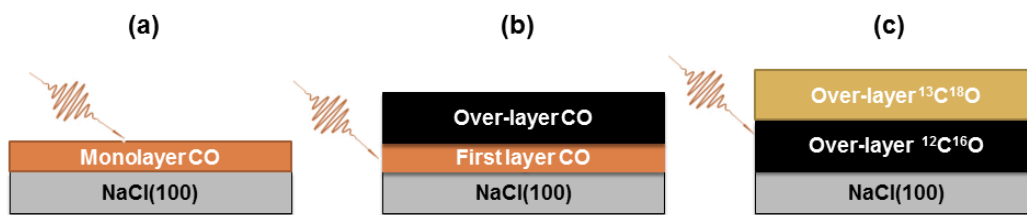


Figure 1 Vibrational dynamics of CO at different interfaces. (a) CO/NaCl (100); (b) CO (overlayer)/CO (first layer)/NaCl (100); (c) $^{13}\text{C}^{18}\text{O}$ / $^{12}\text{C}^{16}\text{O}$ /NaCl (100). At each case, the CO molecules at the layer pointed by the excitation laser pulse are excited. The substrate NaCl(100) surface is kept at 7 K.

Here, I report LIIF study of vibrational dynamics of CO molecules at three solid interfaces (Fig. 1):

- 1) CO/NaCl (100) (Fig. 1a): lateral CO-CO molecular dipole coupling among the CO molecules in the monolayer as well as the CO-NaCl surface phonon coupling;
- 2) CO (overlayer)/CO (first layer)/NaCl (100) (Fig. 1b), vibrational energy flow from the excited first layer CO to the overlayer CO or to the NaCl (100) substrate;
- 3) $^{13}\text{C}^{18}\text{O}$ / $^{12}\text{C}^{16}\text{O}$ /NaCl (100) (Fig. 1c): vibrational energy flow from light CO isotope ($^{12}\text{C}^{16}\text{O}$) to heavy isotope ($^{13}\text{C}^{18}\text{O}$) due to the molecular dipole-dipole coupling, and the interaction range of this dipole coupling.

Modelling non-adiabaticity in thermal recombination reactions on metal surfaces: Transition state theory with dynamical corrections.

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In order to accurately describe atomic scale motion associated with chemical reactions that are relevant to many important industrial processes, the experimentally evidenced non-adiabaticity in gas-surface interactions must be included. Furthermore, to fully characterise the influence of Born-Oppenheimer approximation [1] (BOA) failure on reactions is essential to developing the next generation of predictive theory of surface chemistry. A model systems for which appears likely that electronic coupling can influence reactivity are H₂ recombinative desorption on the Au(111) and Cu(111) surfaces. This systems have a late barrier for dissociation located close to the surface and with large internuclear distance [2]. Such characteristics, as well as current measurements by metal-insulator-metal (MIM) junctions when H atoms interact with Au [3], indicate that electronic excitations might be relevant in the recombination rate constants.

Transition state theory (TST) is undoubtedly the most successful and widely employed theoretical approach for studying reaction rates involving species that undergo reaction at or near thermal-equilibrium conditions. To go beyond the BOA, non-adiabaticity is introduced within the dynamic factor that corrects the TST constant rate. An accurate description of the electronic excitations is accomplished with the recently developed ab-initio molecular dynamics with electronic friction (AIMDEF) method [4]. This method is based on the local density electronic friction (LDEF) [5] method, which was recently shown to successfully model translational energy loss measurements for H colliding with Au(111) [6].

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Molecular Beam Scattering from Ultrathin Metallic Films of Ag/Au(111)

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We investigated the effect of layers of Ag/Au(111) with defined thickness on molecule-surface scattering processes. Beam scattering methods combined with laser-based detection techniques were used to compare these effects for scattering of NO and CO molecules.

Translational energy exchange with ultrathin metallic films of Ag/Au(111) was examined for Ag film thicknesses up to 33 ML at an incidence translational energy of 0.6 eV. For both molecules, we observe a gradual decrease of the mean final translational energy with film thickness for 0 - 3 ML Ag/Au films before reaching a constant value for higher thicknesses. The results are consistent with experimental data for pure Au(111) and Ag(111) crystal surfaces and the comparable thickness dependence of the final translational energy suggests that this kind of inelasticity is purely dominated by mechanical properties of a surface.

Furthermore, we measured the thickness-dependent relaxation probabilities of NO($v = 2$) and CO($v = 2$) scattered from Ag/Au(111). Here, both molecules show a significantly different trend. For NO($v = 2$), relaxation gradually increases between 0-3 ML Ag/Au until reaching a constant value, dominated by multi-quantum relaxation into the vibrational ground state. Comparisons with the work function strongly suggest that this property determines the amount of vibrational energy loss during the collision event. However, for CO($v = 2$), scattering from Au(111) and films above 3 ML Ag/Au(111) exhibit similarly low relaxation probabilities while for a thickness of 1 ML Ag/Au, a maximum of vibrational relaxation into the ground state is observed. In this case, the surface work function does not seem to substantially influence vibrational relaxation, probably due to the low electron affinity of CO (-1.5 eV) in comparison to NO (0.026 eV).

Towards a generalized Effective Medium Theory formalism for H atoms interacting with metals surfaces.

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Recently, detailed theoretical and experimental investigations of energy transfer between hydrogen atoms and late *fcc* transition metal (111) surfaces have been made and on the basis of these experiments, it was possible to clarify the role of electron-hole pair excitation during the scattering process. [1-4] However, those investigative efforts excluded metals that tend to crystallize in other crystal structures, such as body centered cubic (*bcc*) and hexagonal close packed (*hcp*), because the theoretical methods in those investigations are based on Effective Medium Theory (EMT) [5], a theory that has been formulated to describe *fcc* metals and their alloys. Here, I present my first efforts to extend the EMT formalism to describe hydrogen atoms interacting with *bcc* metal surfaces. A hydrogen atom at a W(111) surface has been chosen to serve as a test system. In addition, I will briefly outline further research efforts that are planned in future.

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Threshold Energy and Dynamics of C-H[D] bond Formation on Epitaxial Graphene at Zero Surface Coverage

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C-H bond formation on graphene is highly relevant in many research fields and has been intensively studied for decades. However, two key aspects of the adsorption are still experimentally not known, one which is the adsorption threshold and another which is the energy dissipation characteristics of the newly formed C-H bond. We present experiments on H atom scattering from epitaxial graphene under zero surface coverage. Two separated scattering channels are observed, corresponding to scattered atoms that fail and succeed in crossing the adsorption barrier. Utilizing the dependence of the two scattering channels on the normal incidence energy, the thresholds for initial adsorption are determined: 0.47 ± 0.02 eV for H atom and 0.44 ± 0.06 eV for D atom. Together with *ab initial* molecular dynamics simulations, we show that scattered H atoms that succeed in crossing the barrier lose on average 1 eV energy [half of its incidence energy] in one vibrational period of C-H stretch, pointing to an extremely fast energy dissipation mechanism.

CVD Growth and Properties of 2D Transition Metal Dichalcogenides

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In this talk, I'll present a brief overview of why 2D materials and transition metal dichalcogenides have become one of the hottest fields in chemistry, physics, and materials science. These materials share a common layered structure and chemical formula of MX_2 , where M is a variety of transition metals and X is either S, Se, or Te. I'll present a brief overview of their electronic structure, including an introduction to valley polarization. I'll present some of my lab's recent work in developing strategies for growing high quality crystals of monolayer and few layer TMDCs by chemical vapor deposition, highlighting how the growth of these layered materials differs from the growth of traditional inorganic crystals. Finally, I'll talk about our lab's growth of epitaxial and atomically abrupt interfaces in 2D TMDCs, and how those interfaces can influence the electronic properties of the material.

Hydrogen atom scattering from a free-standing Graphene surface

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We use classical molecular dynamics (MD) simulations to model the scattering of H-atoms from a graphene surface. The Tersoff-Brenner second generation reactive empirical bond order (REBO) potential [1] serves as the global potential energy surface (PES). This general purpose PES can describe the interaction of H with all kinds of carbon orbital hybridizations [2]. It is, however, not accurate enough for our purposes. After reparametrization, we can now reproduce DFT energies with an RMSE of 160 meV. This ensures the reliability of our MD simulations because barrier heights and chemisorption wells are properly described. These decisive features determine whether an incoming H-atom experiences adsorption or reflection.

Our results overall match recent experiments performed by the Bünermann group [3]. The model explains the intensities of the fast and slow peak that the group found in the energy loss spectra which depend on the polar angle of the incident beam. It also describes the very efficient energy transfer between the projectile and the surface that leads to sticking. The REBO PES predicts temperature- and angle- dependent sticking probabilities and a large out of plane contribution to energy loss spectra when the slow component is present.

References

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Associative Desorption of Hydrogen from Coinage Metals

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In this work, the recombinative desorption of hydrogen isotopologues from metal surfaces is studied. Due to the application of a permeation technique the molecule formation mechanism on the single crystal surfaces is restricted to the Langmuir-Hinshelwood reaction of two chemisorbed hydrogen atoms. Quantum state resolved measurements of the product's energy distributions are analyzed using the principle of detailed balance, which yields quantitative information about the dynamics of the reverse process of *dissociative adsorption*. Presented are results for single crystal surfaces of the three coinage metals copper, silver and gold. This formation of the simplest molecule on transition metals with filled *d*-shells constitutes ideal benchmark systems for computational chemistry in surface science. Comparison of our results to such high-level *ab initio* calculations^[1-6] are presented, as well as comparison to other experimental data^[7-12]. These results are then discussed in the light of *chemical accuracy* claimed by theory^[2]. Further results argue for a reevaluation of the non-adiabaticity regularly assumed for this very simple chemical reaction at metal surfaces.

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The “Mobile Beamer”-an atomic and molecular beam surface scattering apparatus for the use at VUV free electron lasers

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The “Mobile Beamer” is designed for surface scattering experiments on atoms and molecules making use of the advantageous properties of the radiation produced by the VUV free electron laser in Dalian (DCLS). The VUV radiation will be used for the production of beams of atoms (O, C, N) in different electronic states by dissociation of small molecules. In addition, the tunable VUV light source can be used for the detection of molecules. As the project is in the late design/early construction phase I would like to discuss our ideas for this project with you at my poster.

Surprisingly long-lived vibrational lifetime of CO on Au(111): A time resolved sum frequency generation study

Sumit Kumar, Dirk Schwarzer and Alec M. Wodtke

Dynamics at Surfaces

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Vibrational lifetime of an adsorbate on a metal surface is of general interest to the scientific community and particularly much relevant in the field of surface science. The reported studies till date demonstrate that the vibrational lifetime of a molecule significantly depends upon the surface properties of substrate. Adsorbate on semiconductor or insulator has vibrational lifetime of few nanoseconds.¹ Vibrational lifetime of excited ($v=1$) state of physisorbed CO on NaCl(100) is in millisecond timescale (~ 4.3 ms).² In contrast, vibrational relaxation of excited ($v=1$) state of strongly bound molecule such as CO on metals (Cu or Pt) takes a few picoseconds (~ 2 ps).^{3,4} Unfortunately, the similar study of vibrational lifetime of weakly bound adsorbate on metal is absent in the literature. Therefore vibrational lifetime measurement of CO on Au(111) has been chosen for the study as Gold, being the noblest metal⁵, prefers weak adsorption of molecules.

In the current work, we have directly measured the vibrational lifetime of CO on Au(111). A newly designed experimental setup has been built to achieve mechanical vibration free surface at low temperature (~ 25 K) for this measurement. We have measured frequency and time domain sum frequency generation spectroscopy using picosecond laser pulses. Spectroscopic measurement of a weakly bound adsorbate-metal system having a low absorption cross-section has been successfully achieved. Vibrational sum frequency generation spectroscopy shows that the stretching vibrational frequency of CO on Au(111) is 2131 cm^{-1} . Interestingly, the current study first time experimentally demonstrates the presence of a comparatively long-lived vibrational state of adsorbate on the metal surface. An IR-pump-probe sum frequency generation spectroscopy shows that the vibrational lifetime of vibrationally excited CO ($v=1$) on Au(111) is 62 ± 10 ps.

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Vibrational Energy Pooling in a CO/NaCl(100) Monolayer: Kinetic Monte Carlo Simulations

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Vibrational energy pooling allows efficient population of highly excited vibrational states via the exchange of vibrational quanta between two molecules (e.g. $\text{CO}(v=n) + \text{CO}(v=m) \rightarrow \text{CO}(v=n+1) + \text{CO}(v=m-1)$). The temporal evolution of each vibrational state after laser excitation can be monitored using time-resolved and dispersed laser-induced infrared fluorescence (LIIF). With a superconducting nanowire single-photon detector (SNSPD), which has been recently used to measure the pooling dynamics of the CO/NaCl(100) multilayer system with unprecedented sensitivity,^[1] we are able to measure dispersed fluorescence from a CO monolayer on NaCl(100) for the first time. Upon pumping the fundamental transition of CO with a short laser pulse (~ 5 ns) at a surface temperature of 7 K, infrared fluorescence originates from $v=4$ up to $v=27$.

In 2002, Corcelli and Tully^[2] proposed a theoretical model to calculate the rate constants for vibrational energy pooling in the monolayer based on LIIF experiments by Chang and Ewing,^[3] who could only measure the total fluorescence. Kinetic Monte Carlo simulations using the original theoretical model fail to reproduce the population in high vibrational states observed in the experiment. By adjusting the model, good agreement with the experimental data is obtained. The key adjustments can be used to extract information on the coupling between CO and the NaCl(100) surface phonons, the electric dipole moment function of CO at the surface, and possible vibrational energy transfer to the first excited electronic state of CO ($V-E$ energy transfer). Combining the highly detailed experimental data and the kinetic simulation thus provides a profound understanding of the energy dissipation and energy transfer dynamics for the CO/NaCl(100) system.

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Scattering of NO from thin film VO₂ surfaces

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Vanadium oxides are among the most used heterogeneous catalysts in industrial applications. Vanadium dioxide (VO₂) is also of interest for the understanding of general interactions between surfaces and gas molecules. It shows a Mott transition at 68°C, at which it changes its electrical properties from insulating to conducting.^[1] Hence, it provides an adjustable band gap to probe non-adiabatic effects governing vibrational energy transfer between molecules and surfaces.^[2,3] This work presents the preparation of VO₂ thin films in a chemical vapor deposition process and subsequent molecule surface scattering experiments.

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Scattering NO from Pt(111) and graphene/Pt(111)

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Scattering small molecules from well-defined surfaces is an exceptional way to investigate energy transfer processes at the gas-solid interface. NO scattering has been performed for different surfaces, such as Ag(111), Au(111) and Ge(111). To this date, there has been little work on small molecule scattering from graphene, a single graphitic layer which can be used as a very sensitive gas detector.

In this work, NO($\nu=0$) and NO($\nu=3$) have been scattered from graphene/Pt(111) synthesized via CVD and from the clean platinum surface. When scattering NO($\nu=3$), nearly no vibrational relaxation is observed on platinum and graphene. On the other hand, vibrational excitation of NO($\nu=0$) is observed on both surfaces. For graphene the NO($\nu=1$) signal increases by a factor of 3.5 whereas it increases by a factor of 5 for the clean platinum surface.

New theoretical methods for chemical dynamics at surfaces

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Chemical reactions at surfaces pose extraordinary challenges from the perspectives of both electronic structure and chemical dynamics. In this talk, I will focus on recent methods, including those based on ring-polymer molecular dynamics [1-3], surface hopping [3], and embedded mean-field theory [4-5], that we have developed to address these challenges and to apply them to both electronically adiabatic and non-adiabatic dynamics at surfaces.

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CO-Oxidation at Platinum

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“CO oxidation is one of the best-known heterogeneous reactions and can thus be regarded as a benchmark system.”

Hans-Joachim Freund, Gerard Meijer, Matthias Scheffler, Robert Schlögl and Martin Wolf,
Angewandte Chemie – International Edition, **2011**.

“...CO oxidation should be considered a benchmark for experiments.”

Alec M. Wodtke, *Wodtke Group Seminar*, **2017**

Challenges and opportunities in C1 chemistry

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C1 molecules include CH₄, CO, CH₃OH and CO₂. In this talk, I will focus mainly on CO, the chemistry of CO conversion to chemicals and fuels. The most challenging is the controlled C–C coupling leading to desired products, for example, ethylene, aromatics and etc, without over-hydrogenation or polymerization to long chain hydrocarbons.^{1,2} We recently reported that coupling of partially reduced oxide surface and confined acidic zeolite pores makes it possible to tune the products of syngas conversion.³⁻⁶ This is enabled by a nanocomposite with bifunctionalities, which affords two types of active sites with complementary properties. The partially reduced oxide surface (ZnCrOx) activates CO and H₂, and C–C coupling is subsequently manipulated within the confined acidic pores of SAPO-34 zeolite. Thus a selectivity of light olefins C₂=–C₄= up to 80% in hydrocarbons is obtained, far beyond that obtained by conventional Fischer-Tropsch synthesis.³⁻⁴ The products can be directed to aromatics with a selectivity up to 74% upon modification of the catalyst.⁶ Characterization with synchrotron-based vacuum ultraviolet photoionization mass spectroscopy (SVUV-PIMS), in situ near ambient pressure X-ray photoelectron spectroscopy (XPS) implied that ketene (CH₂CO) likely plays an important role as an intermediate. These findings open up a new avenue for manipulating the product selectivity in syngas conversion. Some understanding on the mechanism for selectivity control has been gained and is going to be discussed in the presentation.

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Post-permeation associative desorption of hydrogen from a Ag(111) surface

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In this experiment, we used the permeation technique to study the associative desorption of H₂ and D₂ from a Ag(111) surface. Quantum state specific time-of-flight (TOF) distributions were obtained and the principle of detailed balance was applied to extract information about the dissociative adsorption process. Our results are compared to other experimental data^[1-6] which were acquired by a different technique at lower temperatures and to high-level *ab initio* calculations^[7-9]. After copper and gold, we complete our investigation of the associative desorption of hydrogen from the coinage metals. The properties of silver were expected to lie somewhere in between copper and gold^[7]. Contrary to those expectations, the adsorption on silver exhibits an extraordinarily high barrier which strongly depends on the vibrational state while rotational excitation shows almost no effect.

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Investigating mode specificity of nonadiabatic behavior at surfaces

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In recent decades, molecular beam scattering experiments—primarily on diatomic molecules—have demonstrated signatures for distinct mechanisms of vibrationally inelastic energy exchange between molecules and metal surfaces. Namely, mechanical kinetic energy-vibration (T - V) coupling and electronically non-adiabatic electron hole pair-vibration (eHP- V) coupling are both important processes that exhibit qualitatively different dependences on incidence kinetic energy and surface temperature. In polyatomic molecules, these mechanisms might happen simultaneously and mode selectively. Research on diatomic molecules suggests that the eHP- V mechanism involves transient electron transfer from the surface to the molecule, suggesting that the mode selectivity in polyatomics will obey Franck-Condon rules for electron attachment. To look for mode specificity in the electron transfer process, we have scattered formaldehyde, prepared in different vibrational levels of the metastable \tilde{a}^3A_2 electronic state from a low-work function Cs-covered surface and made quantitative measurement of the exo-electrons emitted from the surface. Preliminary results of this experiment will be presented along with measurements of the vibrational and isotopologue dependence of the \tilde{a}^3A_2 dissociative lifetime, which is relevant to below-barrier dissociative tunneling.

Determination of fuchsine-Kaolin:Alginate composite surface interactions: Textile dye remediation from wastewater

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Remediation of textile dyes using polymer layer silicates composite has been used for many publications. In this study biopolymer (Alginate) has been reinforced with layer silicate (kaolin), thereby increasing the adsorption properties of both alginate and kaolin, and to use it as an efficient adsorbent to remove fuchsine dye. In the adsorption of dye molecules-adsorbent surface interactions and interactions between dye molecules are important. Therefore in this study, chemical interactions of adsorbent and the adsorbent surface and the adsorbate-adsorbate interactions will be determined.

All the remediation experiments were conducted using 0.20 g of the composite and 100 mL of 5.0 mg L⁻¹ except for isotherm study where the concentration of fuchsine varied from 0.5-50 mg L⁻¹. Suspensions were shaken on an orbital shaker at a constant speed of 100 rpm.

Composite material adsorbed 93% (2.32 mg g⁻¹) of fuchsine from aqueous system within 240 min. The adsorption process followed pseudo first order kinetic model with a rate constant of 0.023 min⁻¹. Isotherm study showed that the Langmuir-Freundlich combined isotherm model fit the isotherm data with a maximum adsorption capacity of 20.96 mg g⁻¹ and a heterogeneous index value of 1.42. The adsorption is a heterogeneous adsorption process, which forms a layer of fuchsine on the adsorbent surface through chemical bonds and multilayers of fuchsine through hydrogen bonding.

Further studies will be conducted on determination of the adsorbate-adsorbent surface interaction with dye molecules surface scattering and temperature programmed desorption.

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Keywords: Adsorption, Alginate, Fuchsine, Kaolin, molecules beam surface scattering, temperature programmed desorption

Velocity-Resolved Kinetics using Ion Imaging - CO oxidation and trapping at Pt(332) and Pd(111)

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The present work offers a detailed study of the reaction dynamics and kinetics of the CO oxidation and trapping on Pt(332) and Pd(111) by means of molecular beams, spatial ion imaging and velocity-resolved kinetics^[1].

Experiments at Pt(332) and Pd(111) show a bimodality in the kinetic energy distribution of the CO₂ product. While a thermal component is the dominant pathway for the formation of CO₂ at Pt(332), a larger fraction of a hyperthermal CO₂ component contributes to the overall flux at Pd(111). We assign the thermal CO₂ component to be formed at atomic steps and the hyperthermal component to be formed at terraces.

We have previously developed a kinetic mechanism which includes three elementary CO₂ forming reactions at steps and terraces^[2]. We make use of numerical modeling to derive the elementary rate constants for three CO₂ forming reactions at Pt(332) and Pd(111). In contrast to previous studies, we do not find evidence for a coverage dependent activation energy as proposed in previous studies. We claim that these effects result from the fact that previous works were not sensitive for elementary step reactions of CO₂ formation.

We make use of transition state theory and the Serri-Tully-Cardillo model^[3] to get a detailed insight into the nature of the CO desorption process at Pt(332). We find that the overall desorption process is best described by step-assisted desorption and not direct desorption from steps. Furthermore we are able to make an estimation of the CO step-terrace binding energy difference at platinum.

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Scattering highly vibrationally excited CO from a Au(111) surface

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A molecule colliding with the surface of a solid may lose or gain vibrational energy during the collision event. At metal surfaces, electronically non-adiabatic dynamics become important for the vibrational excitation or de-excitation of small molecules. Electronically non-adiabatic dynamics are characterized by a strong coupling between the nuclear motion of the molecule (vibration) and the electronic degrees of freedom of the metal (electron-hole pairs). As the non-adiabatic energy transfer involves an electron transfer from the surface to the molecule, the non-adiabatic propensity of a certain molecule-surface system depends on both the work function of the surface and the electron affinity of the molecule. It has been demonstrated that non-adiabatic effects dominate the energy transfer process when scattering highly vibrationally excited NO from a Au(111) surface because of the high vertical electron binding energy at extended bond lengths. However, NO is the only molecule that has been prepared in high ν states for surface scattering experiments so far. We report on the direct scattering of highly vibrationally excited CO($\nu = 17$) from a clean Au(111) surface. In contrast to NO, highly vibrationally excited CO exhibits a significantly lower vibrational relaxation probability which increases with incidence speed. These findings can be explained by the considerably lower vertical electron binding energy of CO.

Constructing the full-dimensional potential energy surface for the atom-surface interaction using the high-capacity neural network fitting procedure.

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To get an insight and to fully describe the interaction of atoms (mostly hydrogen) with surfaces (e.g. gold and graphene), the existence of an accurate full-dimensional potential energy surface (PES) is crucial. So far the effective medium theory (EMT) has been used to construct a PES by fitting to energy data derived from density functional theory (DFT). The aim of my work is to implement the biologically inspired high-capacity neural network (NN) fitting procedure and use it as an alternative route to fit the DFT energy data producing finally a PES. The NN approach is expected to be more universal and accurate compared to EMT. This is important since the scope of potential application is drastically increased due to the experimental studies recently done in our department.

The NN procedure has already been proven to adequately describe the H@graphene, which makes it possible to effectively simulate the scattering for this system in the large range of incidence conditions.

Increased single-domain size of tungsten disulfide through controlling growth temperature and pretreatment of substrates

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We wish to explore how short-lived electronic excitations in the solid state can influence collisional dynamics, a direction of non-Born-Oppenheimer dynamics that has yet to be explored. Semiconductors are clearly the place to start this type of work as lifetimes of excited electronic states of semiconductors are often on the time scale of our H-atom pulse or longer. Unfortunately, traditional semiconductors like Si present problems. First, excited electron-hole pairs (EHPs) in a bulk semiconductor like Si can clearly be produced by photoexcitation; however, they may not have significant coupling to the H-atom, which is interacting at the surface. This is further complicated by the fact that Si surfaces have dangling bonds and must be passivated - often they are passivated by an oxide. Another problem arises from the fact that Silicon is an indirect band-gap semiconductor, meaning optical transitions are nominally forbidden. The bulk layered materials are indirect band-gap semiconductors; however, inversion symmetry is broken in the monolayer and many transition metal dichalcogenides (TMDs) become direct band-gap semiconductors; they, therefore, interact strongly with light. Choosing monolayers of tungsten disulfide (WS₂) is a particularly interesting way to overcome these problems. WS₂ is a promising material for future nanoelectronics and optoelectronics. It has remained a great challenge to grow large-size crystalline and high surface coverage monolayer WS₂. In this work, we investigate the controllable growth of monolayer WS₂ evolving from triangular flakes to continuous thin films by optimizing the concentration of gaseous WS₂, which has been shown a both thermodynamic and pretreatment growth factor. Previous results, ZnO nanostructure growth has been studied on various substrates through several surface treatments such as UV/Ozone and plasma. After UV/Ozone treatment, the density of nanostructure has been increased a hundredfold and uniformity of diameter has been improved as well. The increase in WS₂ size can be explained by the enhanced nucleation probability and the growth velocity, caused by the additional precursors supplied during the rapid cooling.

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