

## O 46: Electron-Driven Processes at Surfaces and Interfaces

Time: Wednesday 10:30–12:15

Location: CHE 91

O 46.1 Wed 10:30 CHE 91

**On the energy transfer mechanism in hyperthermal H atom scattering from surfaces** — ●NILS HERTL<sup>1</sup>, CONNOR L. BOX<sup>1</sup>, and REINHARD J. MAURER<sup>1,2</sup> — <sup>1</sup>Department of Chemistry, University of Warwick, UK — <sup>2</sup>Department of Physics, University of Warwick, UK

Adsorption of atomic and molecular hydrogen on surfaces is the gateway to many important chemical processes in nature. Hence, it is important to understand their adsorption mechanism if we want to understand the relevant elementary processes of these adsorbates on surfaces.

In the recent years, a series of detailed theoretical and experimental investigations of energy transfer between H atoms and a variety of material surfaces have been performed. The investigated substrates range from noble gas surfaces with a detour to semiconductors to late fcc transition metal surfaces. Transition metal surfaces with adsorbates were investigated, too. For all studies, a UHV apparatus, specifically designed for H atom scattering, has been used. The complementary theory relies on molecular dynamics simulation, where electronic excitations are described within the framework of molecular dynamics with electronic friction. The friction coefficient is treated within the local density friction approximation (LDFA).

In this talk, I will briefly revisit those studies and on the basis of them, I will formulate a couple of general concepts relevant to atom scattering from surfaces. Furthermore, I will also present first efforts to apply methods which go beyond the framework of LDFA friction for hyperthermal H atom scattering.

O 46.2 Wed 10:45 CHE 91

**Simulations of H atom scattering from p(2×2) O/Pt(111) surface with orbital-dependent friction** — ●CONNOR L. BOX<sup>1</sup>, NILS HERTL<sup>1</sup>, and REINHARD J. MAURER<sup>1,2</sup> — <sup>1</sup>Department of Chemistry, University of Warwick, United Kingdom — <sup>2</sup>Department of Physics, University of Warwick, United Kingdom

The experimentally recorded nonadiabatic energy loss that occurs during H atom scattering from a range of clean metal surfaces is well reproduced by the molecular dynamics with electronic friction method using effective medium theory for the potential energy surface and the local-density friction approximation for the electronic friction. [1] However, it was recently reported that this method is not capable of reproducing the inelastic scattering of H atoms on the oxygen-covered Pt(111) surface. [2] We present inelastic scattering energy loss distributions for this system with an efficient ML representation of the orbital-dependent friction coefficients calculated using linear response theory based upon density functional theory. This approach additionally accounts for the anisotropy of the electronic friction tensor and the effect of the oxygen adatom on the surface electronic structure. [1] Dorenkamp et al, JCP, 2018 [2] Lacroart et al, JCP, 2021

O 46.3 Wed 11:00 CHE 91

**Power discontinuity and shift of the energy onset of a molecular de-bromination reaction induced by hot-electron tunneling** — ANA BARRAGAN<sup>1</sup>, ROBERTO ROBLES<sup>1</sup>, NICOLAS LORENTE<sup>1,3</sup>, and ●LUCIA VITALI<sup>1,2,3</sup> — <sup>1</sup>Centro de Física de Materiales CFM/MPC (CSIC-UPV/EHU), San Sebastián, Spain — <sup>2</sup>Ikerbasque Research Foundation for Science, Bilbao Spain — <sup>3</sup>Donostia International Physics Center (DIPC), San Sebastian

Understanding the mechanism of molecular dissociation under applied bias is a fundamental requirement to progress in (electro)-catalysis as well as in (opto)-electronics. The working conditions of a molecular-based device and the stability of chemical bonds can be addressed in metal\*organic junctions by injecting electrons in tunneling conditions. Here, we have correlated the energy of debromination of an aryl group with its density of states in a self-assembled dimeric structure of 4'-bromo-4-mercaptobiphenyl adsorbed on an Au(111) surface. We have observed that the electron-energy range where the molecule is chemically stable can be extended, shifting the bias threshold for the rupture of the -C-Br bond continuously from about 2.4 to 4.4 V by changing the electron current. Correspondingly, the power needed for the dissociation drops sharply at 3.6 V, identifying different reaction regimes and the contribution of different molecular resonance states.

A.Barragan, R.Robles, N.Lorente, L.Vitali; Nanoscale 13, 15215 (2021)

O 46.4 Wed 11:15 CHE 91

**Quantum transport on anisotropic surfaces revealed by MONA** — ●MANUEL SEITZ<sup>1</sup>, ANDREAS CHRIST<sup>1</sup>, MARKUS LEISEGANG<sup>1</sup>, JACEK WALUK<sup>2</sup>, and MATTHIAS BODE<sup>1</sup> — <sup>1</sup>Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — <sup>2</sup>Institute of Physical Chemistry, Polish Academy of Sciences, ul. Kasprzaka 44/52, 01-224 Warsaw, Poland

The ability to detect how charge carriers propagate in well-defined bands is of great importance for the exploitation of novel materials, e.g., in the context of spintronics or topological insulators. We developed the molecular nanoprobe (MONA) technique [1] to investigate the details of quantum transport. It utilizes a single molecule to detect ballistic charge carriers injected by the tip of a scanning tunneling microscope (STM). In this study, we investigate charge carrier transport in the structurally anisotropic Cu(110) surface which exhibits a surface state at the Y-point of the surface Brillouin zone [2]. We performed directional-, distance-, and energy-dependent measurements that reveal an unexpectedly rich anisotropic behavior. The results can be explained by the combined influence of the band structure-dependent transport path and the molecular excitation.

[1] Leisegang, M. et. al., Nano Lett. 18, 2165 (2018).

[2] Jiang, J., et. al., Phys. Rev. B 89, 085404 (2014).

O 46.5 Wed 11:30 CHE 91

**Understanding triplet-exciton transfer dynamics at the Si-tetracene interface** — ●MARVIN KRENZ — Universität Paderborn

Singlet-exciton fission in a tetracene overlayer and the subsequent triplet-exciton transfer into a silicon solar cell appears as promising approach to harvest high-energy photons [1]. However, the details of the exciton transfer and its dependence on the interface atomic structure are not understood. In the present contribution we employ ab initio non-adiabatic molecular dynamics to study the exciton transfer in atomistic detail. It is found that interface defects as well as thermal activation are instrumental for the exciton transfer from the organic overlayer into the Si bulk material.

[1] J.M. Luther, J.C. Johnson, Nature 571, 38 (2019)

O 46.6 Wed 11:45 CHE 91

**Uni-directional translation of a novel adsorbate motor** — ●GRANT J. SIMPSON<sup>1</sup>, MATS PERSSON<sup>2</sup>, and LEONHARD GRILL<sup>1</sup> — <sup>1</sup>University of Graz, Graz, Austria — <sup>2</sup>University of Liverpool, Liverpool, UK

Molecular motors are fascinating objects that can undergo uni-directional motion on the nanoscale. In order to independently perform meaningful work, they typically must switch between two potential energy surfaces to achieve directed motion. However, their rather complex structures often mean that their function on a surface is hindered. Here, we present a novel 'adsorbate motor' which performs strictly uni-directional translational upon excitation from the tip of a scanning tunneling microscope - in contrast to thermally induced motion of the same molecules that follows the principle of microscopic reversibility, resulting in random movement. The resulting 100% uni-directionality is then harnessed in order to perform meaningful work exemplified by the transport of single molecules across a metal surface.

O 46.7 Wed 12:00 CHE 91

**Extreme magnetoresistance in high-mobility Al<sub>2</sub>O<sub>3</sub>/SrTiO<sub>3</sub> heterostructures** — ●DENNIS CHRISTENSEN — Technical University of Denmark, Department of Energy Conversion and Storage, 2800 Kgs Lyngby, Denmark

The heterostructure formed by depositing spinel  $\gamma$ -Al<sub>2</sub>O<sub>3</sub> on perovskite SrTiO<sub>3</sub> exhibits a range of exciting properties including room temperature epitaxial growth [1,2], high electron mobility [3,4], a strain-tunable magnetic order [5] and a reordering of the  $t_{2g}$  bands due to the broken symmetry at the spinel/perovskite interface [6]. Here, I explore the magnetotransport properties of  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>/SrTiO<sub>3</sub> and show that it exhibits a very large magnetoresistance exceeding 80,000% at 16 T and 2 K. When increasing the magnetic field, the field dependence of the magnetoresistance transitions from quadratic to linear with no saturation observed up to 16 T. I discuss the origin of this behaviour in relation to mechanisms known to produce large, unsaturated magne-

toresistance.

[1] M. von Soosten, D. V. Christensen et al. *Scientific Reports* 9, 18005 (2019).

[2] Y. Z. Chen et al. *Advanced Materials* 26, 1462 (2014).

[3] Y. Z. Chen, N. Bovet, F. Trier, D. V. Christensen, et al. *Nature*

*Communications* 4, 1371 (2013).

[4] D. V. Christensen, et al. *Physical Review Applied* 9, 054004 (2018).

[5] D. V. Christensen, et al. *Nature Physics* 15, 269 (2019).

[6] A. Chikina, D. V. Christensen et al. *ACS Nano* 15, 4347 (2021).