Symposium Molecular Switches and Motors at Surfaces (SYMS)

jointly organized by
Surface Science Division (O),
Biological Physics Division (BP), and
Chemical and Polymer Physics Division (CPP)

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Overview of Invited Talks and Sessions

(Lecture room: HSZ 02)

Invited Talks

SYMS 1.1	Wed	9:30–10:00	HSZ 02	**Imaging and manipulation of single functional molecules on surfaces** — •Leonhard Grill
SYMS 1.2	Wed	10:00–10:30	HSZ 02	**Adiabatic quantum motors** — •Felix von Oppen
SYMS 1.3	Wed	10:30–11:00	HSZ 02	**Operation of molecular devices and machines on surfaces** — •Saw Wai Hla
SYMS 1.4	Wed	11:15–11:45	HSZ 02	**Driving and Controlling Molecular Surface Rotors with a Terahertz Electric Field** — •Raymond Dean Astumian
SYMS 1.5	Wed	11:45–12:15	HSZ 02	**Unidirectional motion by inelastic electron tunneling** — •Karl-Heinz Ernst

Sessions

SYMS 1.1–1.5	Wed	9:30–12:15	HSZ 02	**Molecular Switches and Motors at Surfaces**

SYMS 1: Molecular Switches and Motors at Surfaces

Time: Wednesday 9:30–12:15 Location: HSZ 02

Invited Talk SYMS 1.1 Wed 9:30 HSZ 02

Imaging and manipulation of single functional molecules on surfaces — •Leonhard Grill — University of Graz, Department of Physical Chemistry, Graz, Austria

Functional molecules on surfaces and their assembly into pre-defined architectures are key challenges in nanotechnology and of interest in various fields from molecular electronics over novel materials to molecular machines. Various examples of functional molecules, studied by scanning tunneling microscopy under ultrahigh vacuum conditions will be discussed. Specifically designed molecular building blocks are connected to two-dimensional networks or one-dimensional chains [1,2], which can act as molecular wires [3,4]. On the other hand, chemical processes within individual molecular can be controlled via their environment. This was observed for molecular switches, where the atomic-scale surroundings cause drastic changes in their switching probability [5]. Recently, we could show that the rate of an intramolecular hydrogen transfer reaction can be tuned up and down by single atoms in the vicinity of the molecule [6]. Finally, a combination of the two approaches will be discussed, potentially leading to heterogeneous molecular nanostructures that contain functional molecules.

[1] L. Grill et al., Nature Nanotech. 2, 687 (2007); [2] L. Lafferentz et al., Nature Chem. 4, 215 (2012); [3] L. Lafferentz et al., Science 323, 1193 (2009); [4] M. Koch et al., Nature Nanotech. 7, 712 (2012); [5] C. Dri et al., Nature Nanotech. 3, 649 (2008); [6] T. Kumagai et al., Nature Chem., doi: 10.1038/nchem.1804.

Invited Talk SYMS 1.2 Wed 10:00 HSZ 02

Adiabatic quantum motors — •Felix von Oppen — Dahlem Center for Complex Quantum Systems, Freie Universität Berlin

Microscopically, motion is frequently dominated by fluctuations, making it a challenge to generate directed motion at the nanoscale. This challenge has motivated recent experiments striving to realize nanomotors which convert electrical signals into unidirectional translational, vibrational, or rotational motion. Frequently, these experiments rely on ac actuation or current pulses to effect the directed motion of, say, a molecule or a carbon nanotube. In this talk, I will describe an alternative dc scheme to operate a nanomotor. Our proposed adiabatic quantum motor is effectively based on operating a quantum pump in reverse, a scheme whose macroscopic counterpart has been known since antiquity and is employed in current technology. Its quantum version has remained essentially unstudied despite enormous activity on adiabatic quantum pumps. Specifically, we consider a transport current which drives the periodic motion of an adiabatic degree of freedom. We relate the work performed per cycle on the motor degree of freedom to characteristics of the complementary quantum pump and discuss the motors' efficiency. We show that in principle, there exist motors which operate solely due to quantum interference, as well as ideal quantum motors with unit efficiency. The intrinsic damping of quantum motors has a lower bound which just involves Planck's constant. While most of our considerations are based on Gedankenmotors, we will also discuss possible realizations.

Invited Talk SYMS 1.3 Wed 10:30 HSZ 02

Operation of molecular devices and machines on surfaces — •Saw Wai Hla — Center for Nanoscale Materials, Argonne National Lab, and Ohio University, USA.

A recent emergent research direction is the development of complex molecular machines suitable to operate on solid surfaces. Unlike biological counterparts, the synthetic molecular machines may tolerate a more diverse range of conditions, and thus be advantageous for the complex functions with low power consumption suitable to operate in solid state devices. Development of such molecular devices requires testing their operation mechanisms. We use low temperature scanning tunneling microscopy, spectroscopy, and molecular manipulation schemes to investigate fundamental operations of synthetic molecular switches and molecular motors on metallic surfaces. Using inelastic electron tunneling process, individual molecules can be switched from one state to another in a controlled manner [1-4]. Controlled directional rotation of molecular motors can also be performed using the same technique. Finally, this presentation will include our latest results of controlled synchronized rotation of molecular motors on surfaces.

[1] V. Iancu, A. Deshpande, S.-W. Hla, Nano Lett. 6, 820-823 (2006). [2] V. Iancu, and S.-W. Hla, Proc. Nat. Acad. Sci. 103, 13718-13721 (2006). [3] Y.-S. Fu et al. Nano Lett. 12, 3931-3935 (2012). [4] U.G.E. Perera et al. Nature Nanotechnology 5, 46-51 (2013).

15 min. break

Invited Talk SYMS 1.4 Wed 11:15 HSZ 02

Driving and Controlling Molecular Surface Rotors with a Terahertz Electric Field — •Raymond Dean Astumian — Dept. of Physics, University of Maine, USA

Great progress has been made in the design and synthesis of molecular motors and rotors. Loosely inspired by biomolecular machines such as kinesin and the FoF1 ATPsynthase, these molecules are hoped to provide elements for construction of more elaborate structures that can carry out tasks at the nanoscale corresponding to the tasks accomplished by elementary machines in the macroscopic world. Most of the molecular motors synthesized to date suffer from the drawback that they operate relatively slowly (less than kHz). Here we show by molecular dynamics studies of a diethyl sulfide rotor on a gold(111) surface that a high- frequency oscillating electric field normal to the surface can drive directed rotation at GHz frequencies. The maximum directed rotation rate is 1010 rotations per second, significantly faster than the rotation of previously reported directional molecular rotors. Understanding the fundamental basis of directed motion of surface rotors is essential for the further development of efficient externally driven artificial rotors. Our results represent a step toward the design of a surface-bound molecular rotary motor with a tunable rotation frequency and direction.

Invited Talk SYMS 1.5 Wed 11:45 HSZ 02

Unidirectional motion by inelastic electron tunneling — •Karl-Heinz Ernst — Empa, Swiss Federal Laboratories for Materials Science and Technology — Department of Chemistry, University of Zurich

Propelling single molecules in a controlled manner along an unmodified surface remains extremely challenging because it requires molecules that can use light, chemical or electrical energy to modulate their interaction with the surface in a way that generates motion. Biomolecular motors, such as the protein kinesin or the F1-ATPase, function as linear walkers or rotary motors. Chemists strive for synthesis of molecules that can perform unidirectional motion on surfaces. One successful approach was the use of ratchet-style unidirectional rotors based on overcrowded helical systems.

We show that excitation with inelastically tunneling electrons emanating from the tip of a scanning tunneling microscope (STM) very efficiently excites the rotors and leads to linear movement of the molecule on the surface for the right isomer. This requires a transient electron attachment into the LUMO, while vibronic excitation of the motor axles lead to reversible rearrangement without movement. We will discuss possible mechanisms and implication for further research and design of nanotechnological devices.