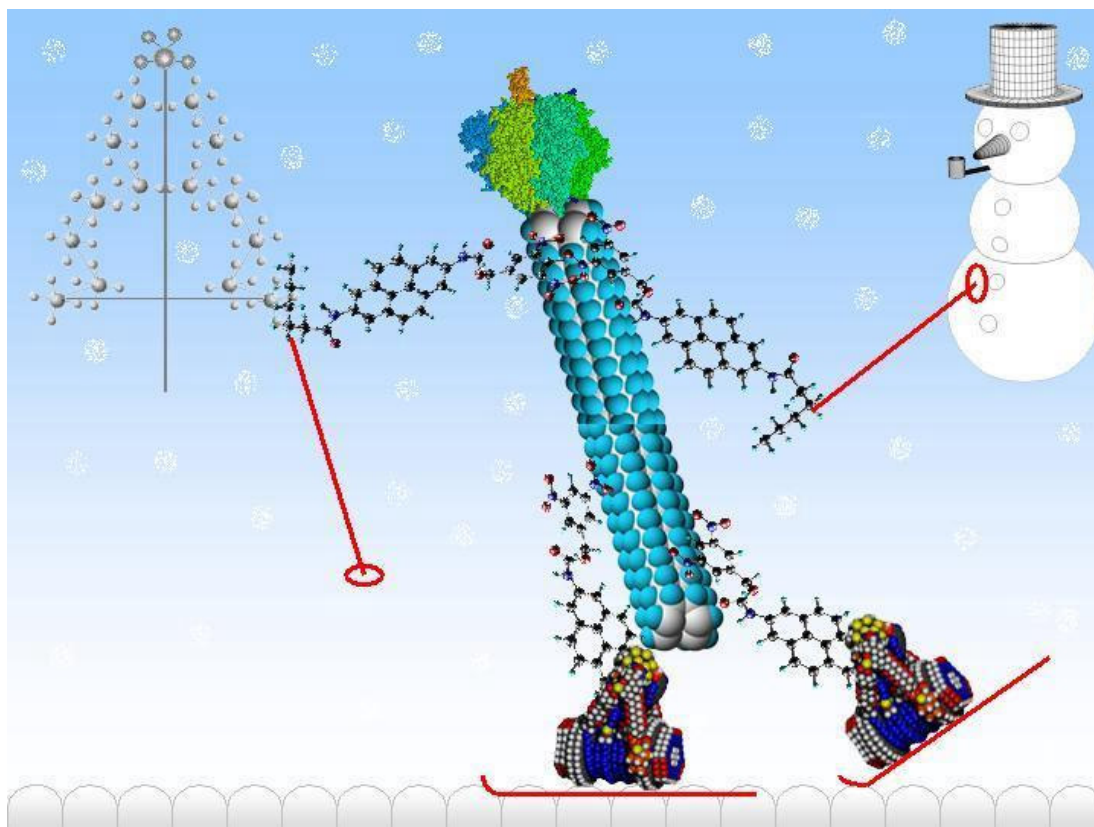


**Research Conference within the European RTN network « Atomic and Molecular Manipulation : a new tool in Science and Technology » (AMMIST)**

# **Molecular Nano-Machines**

**17-21 January 2005**



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**Research Conference on**

*Molecular Nano-machines*

Centre of Physics, Les Houches, France

<http://www-houches.ujf-grenoble.fr/>

**17-21 January 2005**

*The conference is organized in the frame of the European RTN network*

*« Atomic and Molecular Manipulation : a new tool In Science and Technology »*

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These contributions are greatly appreciated and made possible additional invited speakers and participants.

## **Research Conference on**

*Molecular Nano-machines*

Centre of Physics, Les Houches, France

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### **Scope of the conference**

*The manipulation of individual atoms and molecules with the Scanning Tunneling Microscope (STM) has opened up fantastic perspectives in many fields of science and technology. Recently a new concept has emerged where atoms and molecules are considered not only as elementary building blocks of matter but moreover as nano-objects or nano-machines in themselves. Using a single molecule as a functionalized nano-machine will require being able to control not only the position but also numerous geometric, electronic, chemical and mechanical parameters at the atomic level. This concept of molecular nano-nanomachines is also relevant in chemistry and biology where functionalized molecules can be synthesized and manipulated.*

*The goal of the conference is to review recent experimental and theoretical advances in the field of molecular nano-machines in physics, chemistry and biology.*

**Research Conference on**

*Molecular Nano-machines*

Centre of Physics, Les Houches, France

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**17-21 January 2005**

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# Final Program

Monday January 17

**8:30 Opening**, G. Dujardin, *Université Paris-Sud*

**Chair**, Gerhard Meyer

**8 :40 Design and chemical synthesis of a Cu(111) surface wave unimolecular Morse manipulator**

C. Joachim and F. Thieman, *CEMES (France)*

**9 :25 Picometer-scale electronic control of molecular dynamics inside a single molecule**

M. Martin, *Université Paris-Sud (France)*

**10 :10 - COFFEE BREAK-**

**Chair**, Richard Palmer

**10 :40 Scanning Tunneling Microscopy of single atoms and molecules on ultrathin insulating films**

J. Repp, *IBM Zurich Research Laboratory (Switzerland)*

**11 :25 DFT simulations of STM and STS of Cl vacancies in ultrathin NaCl films on Cu**

S. Paavilainen, *Chalmers (Sweden)*

**12 :15 - LUNCH-**

**16 :30 Mid-term-review meeting of the AMMIST network**  
(restricted participation)

**19 :30 - DINNER-**

**Chair**, André Gourdon

**20 :30 Manipulation signal and intramolecular deformation of a 4-legs molecule during its STM manipulation on a Cu(211) surface**

M. Alemani, *FUB (Germany)* and X. Bouju, *CEMES (France)*

**21 :15 Spontaneous and directed assembly of molecular nanostructures**  
P. Beton, University of Nottingham (*UK*)

**Tuesday January 18**

**8 :30 Mid-term-review meeting of the AMMIST network**  
(restricted participation)

**Chair,** Mats Persson

**10 :30 Single molecule desorption and dissociation at room temperature**  
R. Palmer, University of Birmingham (*UK*)

**11 :15 Molecular and supramolecular assembly and positioning at surfaces**  
T. Jung, Paul Scherrer Institute (*Switzerland*)

**12 :15** **-LUNCH-**

**19 :30** **-DINNER-**

**Chair,** Andrew Mayne

**20 :30 Cu(111) surface waves created by the Lander series molecules**  
L. Gross, FUB (*Germany*) and C. Joachim, CEMES (*France*)

**21 :15 Prototypes of artificial molecular machines and motors**  
A. Credi, Universita du Bologna (*Italy*)

## Wednesday January 19

**Chair, Philippe Dumas**

**8 :30 Semiconductor nano-crystals for photon nano-sources**

R. Bernard, Université Paris-Sud (*France*)

**9 :15 Organic nanofibers**

K. Al-Shamery, University of Oldenburg (*Germany*)

**10 :00 - COFFEE BREAK -**

**Chair, Jean-Pierre Galaup**

**10 :30 Tracking individual proteins in live cells using semiconductor quantum dots**

M. Dahan, ENS (*France*)

**11 :15 Functional molecules and transition metal complexes for molecular machines**

V. Huc, Université Paris-Sud (*France*)

**12 :15 - LUNCH -**

**19 :30 - DINNER-**

**Chair, Claudia Veigel**

**20 : 30 How the cell converts energy**

G. Cappello, Institut Curie (*France*)

**21 : 15 How two-foot molecular motors may walk**

K. Kinosita, Okazaki Institute for Integrative Bioscience (*Japan*)

## Thursday January 20

**Chair**, Georges Raseev

**8 :30 Nano-manipulation with Laser+STM**

D. Riedel, Université Paris-Sud (*France*)

**9 :15 Double well unimolecular effect : Photochromism and electrochromism in a molecule**

C . Coudret, CEMES (*France*)

**10 :00 - COFFEE BREAK -**

**Chair**, Katharina Al-Shamery

**10 :30 Ordering and dynamics for a family of oligo(phenylene ethynylene)s on Au(111) studied by UHV-STM**

T.R. Linderoth, University of Aarhus (*Denmark*)

**11 :15 Scanning Probe Energy Loss Spectroscopy**

A. Pulisciano, University of Birmingham (*UK*)

**12 : 15 - LUNCH -**

**19 : 30 - DINNER-**

**Chair**, Thomas Jung

**20 :30 Single molecule mechanics of myosin motors using optical tweezers**

C. Veigel, NIMR (*UK*)

**21 :15 Listening to atoms in atom manipulation and autonomous atom assembly**

J. Stroscio, NIST (*USA*)

## Friday January 21

**Chair**, Elizabeth Boer-Duchemin

**8 :30 The IBM Nanostencil : Design and first experiments**

P. Zahl, IBM Zurich Research Laboratory (*Switzerland*)

**9 :15 Dynamics and self-assembly of organic adsorbates on single-crystal metal surfaces**

R. Otero, University of Aarhus (*Denmark*)

**10 :00 - COFFEE BREAK -**

**Chair**, Joseph A. Stroscio

**10 :30 Assembly of chemical modules under physical constraints : a road to engineer biological complexity ?**

L. Jullien, ENS (*France*)

**11 :15 Changing the conformation of single molecules by manipulation with the STM tip**

L. Grill, FUB (*Germany*)

**12 : 15 - LUNCH -**

**- END -**

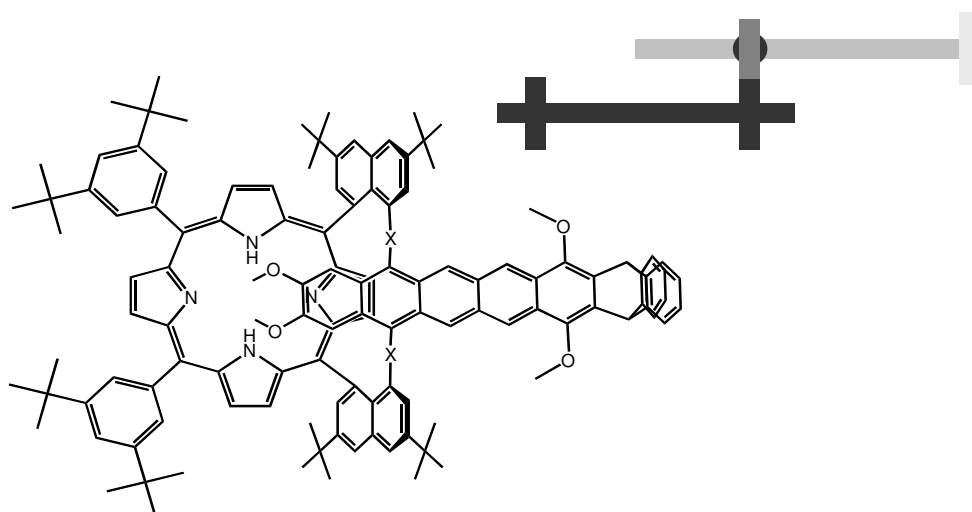
## Design and chemical synthesis of a Cu(111) surface wave unimolecular Morse manipulator

F. Thiemann, C. Joachim, C. Wang, and G. Rapenne

NanoSciences Group, CEMES, UPR 8011 CNRS, Toulouse France

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During the last years enormous efforts in nanotechnology and surface science have been made.<sup>[1]</sup> After it was realized that one can image and manipulate single atoms on a surface using STM techniques, the interest was focused on manipulation of single and large molecules on metallic surfaces.<sup>[2,3]</sup> Following the finding that a conjugated molecule maintained in a physisorption states on a Cu(111) metallic surface can serve as a surface wave scattering center,<sup>[4]</sup> we have now designed a series of molecules equipped with an arm holding a conjugated end group. By the similarity with the first Morse telegraph, our *Morse* molecule was designed in such a way that it can be manipulated on a metal surface due to its 4 legs and that the arm can be manipulated up and down the surface for the end conjugated part to modulate the standing wave patterns of a Cu(111) surface.



The molecular mechanics and the design of the series of *Morse manipulator* molecules will be presented leading to our first synthetic results. Consequences for the synthetic strategy will be discussed.

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- [3] F. Moresco, G. Meyer, K.H. Rieder, H. Tang, A. Gourdon and C. Joachim *Appl. Phys. Lett.*, 78, 306 (2001).
- [4] L. Gross, F. Moresco, L. Savio, A. Gourdon, C. Joachim and K.H. Rieder, *Phys. Rev. Lett.*, 93, 056103 (2004)

## **Electronic control of molecular dynamics inside a bistable molecule**

M.G. Martin, M.J. Lastapis, D. Riedel, L. Hellner, G. Comtet and G. Dujardin

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Bât 210 Université Paris Sud 91405 Orsay Cédex

Although a range of technologies exists for fabricating nanostructures, a very promising method is single molecule engineering with the scanning tunnelling microscope (STM). The tip of a STM can be used to fabricate and to operate nanometre scale molecular structures by electronic or quantum control of single molecules adsorbed on semiconductor surfaces. Thus, the STM offers exciting perspectives for operating molecular nanomachines. Unlike metals, semiconductors have a forbidden gap. By carefully selecting adequate molecules with smaller energy gaps than the semiconductor substrates it will be possible to efficiently enhance the electronic excitation processes that will allow the triggering of a number of functions at the molecular level such as configuration transformations, lateral movement, fluorescence, etc. The system we have studied is the biphenyl molecule adsorbed on a Si(100) surface. This system can be considered as a prototype of an atomic-scale switch. At low temperature (5K), the molecule behaves as a bistable molecule which can be rotated in a reversible fashion from one stable configuration to the other by electronic excitation with electrons from the STM tip. The ability of the STM to perform experiments inside a single molecule has allowed us to excite the two phenyl groups and the silicon substrate separately. By doing so, we have found the existence of a transient molecular configuration that the molecule adopts when oscillating between the two bistable sites. This third configuration is stable enough to be monitored by STM. Based on these capabilities for controlling the electronic excitation and the ensuing molecular dynamics in real space with sub-molecular precision, a new quantum technology inside single molecules can be envisaged for fabricating and operating molecular nanomachines or computing devices.

**Scanning-tunneling microscopy of single atoms and molecules  
on ultrathin insulating films**

J. Repp and G.Meyer

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Adsorbates on metal surfaces are strongly disturbed in their intrinsic properties by the presence of the substrate electrons. Recent progress in carrying out scanning tunneling microscopy and spectroscopy of individual adsorbates on ultrathin, insulating films supported by metal surfaces has therefore opened up a new fascinating field in atomic-scale science.

Individual gold atoms adsorbed on ultrathin insulating NaCl films on copper exhibit two different charge states, which are stabilized by the large ionic polarizability of the film. The charge state and associated physical and chemical properties such as diffusion can be controlled by adding or removing a single electron to or from the adatom with a scanning tunneling microscope tip. Pentacene molecules on NaCl films, on the other hand, preserve their inherent electronic structure that can now be studied by means of scanning tunneling microscopy. Thereby direct images of the unperturbed molecular orbitals of individual pentacene molecules are obtained.

## DFT simulations of STM and STS of Cl vacancies in ultrathin NaCl films on Cu

Sami Paavilainen, Fredrik Olsson and Mats Persson,  
*Department of Applied Physics, Chalmers/GU, Gothenburg, Sweden*

The recent progress in carrying out scanning tunnelling microscopy and spectroscopy of adsorbates on ultrathin, insulating films supported by metal surfaces has opened up a new fascinating field in the atomic scale science and has revived the interest in double-barrier tunnelling junctions. Examples of new physical insights and phenomena obtained from such studies are control of the charge state of adatoms [Repp *et al.*, *Science* **305**, 493 (2004)], single-atom spin-flip spectroscopy [Heinrich *et al.*, *Science* **306**, 466 (2004)], and vibronic states and bipolarity in single molecule transport [Qiu *et al.*, *Phys. Rev. Lett.* **92**, 206102 (2004)]. All these phenomena depend critically on the electronic decoupling of adsorbate-induced states from the metal substrate states by the film. In the typical case of polar, insulating film, there is also another interesting effect, the large electron-phonon coupling found in the tunnelling.

An ideal model system for the study of tunnelling through a localized electronic state on an ultrathin, insulating film is provided by a Cl vacancy in NaCl layers on Cu surfaces. We have carried out density functional theory (DFT) calculations of Cl vacancies in ultrathin NaCl films on Cu(311) and Cu(100) and simulated scanning tunnelling microscope (STM) images and  $dI/dV$  spectra using the Tersoff-Hamann scheme. An F-center state is found to be localized at the vacancy site but is unoccupied in contrast to bulk NaCl F-centers. The simulated STM image is in excellent agreement with experiments with the Cl vacancy seen as a missing protrusion while the nearest neighbour Cl ions are seen as higher protrusions than other Cl ions due to their outward relaxations. The simulated  $dI/dV$  spectra show F-center states at lower energies than the corresponding peaks in experimental  $dI/dV$  spectra, which is an expected shortcoming in the DFT calculations. To improve on this, we have implemented an extension to the DFT to describe negative ion resonance (NIR) states, as the singly occupied F-center state is in this case. The total energy difference between NIR and ground state should then correspond to the peaks seen in the  $dI/dV$  spectra, and this is found to be in much better agreement with experimental data. Furthermore, the geometrical optimization of the NIR from the ground state ion configuration shows a large relaxation energy indicating a strong coupling of the tunnelling electron with the phonons in NaCl films. This explains the broad Gaussian lineshape of the F-center state found in the experimental  $dI/dV$  spectra.

We plan also to present work in progress on divacancies in the NaCl bilayers on Cu(311) which are found to form symmetric and anti-symmetric molecular orbitals with a rather large energy splitting. We have also work in progress concerning NIR states of Au monomers and dimers on the NaCl layers on Cu(100).

## **Manipulation signal and intramolecular deformation of a 4-legs molecule during its STM manipulation on a Cu(211) surface**

X. Bouju, M. Alemani, C. Wang, L. Gross, F. Moresco and C. Joachim  
Speakers: (1) M. Alemani and (2) X. Bouju

A detailed Low-Temperature Scanning Tunneling Microscope study of the controlled manipulation of a Lander molecule  $C_{90}H_{98}$  adsorbed on Cu(211) is presented. Simulations based on detailed elastic scattering quantum chemistry description combined with molecular mechanics calculations are performed to reproduce the STM current during the manipulation.

We demonstrate that the main tunnelling current is flowing through the central molecular wire even if the STM tip is pushing on a leg of the Lander molecule.

This is due to the fact that the intramolecular deformation induced by the manipulation opens other tunneling paths which are not directly located on the point of the molecule in close contact with the tip apex.

## Spontaneous and directed assembly of molecular nanostructures

Peter Beton

University of Nottingham (UK)

The positioning of molecules on semiconductor surfaces using the tip of a scanning tunnelling microscope and also through exploitation of directional intermolecular interactions such as hydrogen bonding is discussed. The response of fullerene molecules to translational displacement across a Si(100)-2x1 surface has been measured and a long range periodic response is observed. This corresponds to a molecular sequentially adopting a series of different adsorption states which we identify as different rotational configurations. The periodic adoption of these states implies that the translational and rotational motion of the fullerene is strongly coupled. We propose a model for the response of the molecule in which rotation and translation are intimately coupled through a motion in which the molecule pivots over a pair of unbroken bonds. This model is supported by numerical calculations [collaboration with Kantorovich and Hobbs, Kings College London] and has been extended to account for a range of other responses with different periodicities and subharmonic features. We also describe recent work in which PTCDI and melamine molecules spontaneously form a two dimensional network which is stabilised by hydrogen bonding. The network can be used as a template which can capture further adsorbed molecules and we present results on the growth of higher fullerene clusters on such a network. This work shows that molecules grown within a confined nanoscale geometry can adopt new cluster configurations and ordering which is not observed in bulk phases.

# Single Molecule Desorption and Dissociation at Room Temperature

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Bond-selective molecular manipulation is one of the frontiers of atomic manipulation with the STM. Traditionally such experiments are conducted in the stable, low temperature regime; room temperature manipulation is much more challenging. Here we demonstrate room temperature, bond selective manipulation (“molecular dissection”) in a polyatomic molecule - chlorobenzene ( $C_6H_5Cl$ ) anchored to the Si(111)- $7\times 7$  surface by chemisorption. Recently we showed that the mechanism of electron (or hole) injection from the STM tip into the  $\pi^*$  LUMO (or  $\pi$  HOMO) orbitals of the benzene ring leads to controlled molecular desorption beyond a threshold voltage of +2.5V (-1.5V) [1]. The desorption yield is linearly proportional to the STM junction current, indicating a one electron process. In this work we explore C-Cl bond dissociation in the chemisorbed chlorobenzene molecule. Detailed STM images allow us to identify the azimuthal orientation of the individual chlorobenzene molecules on the surface and thus to correlate the final location of the liberated chlorine “daughter” atom with the position and orientation of the parent molecule [2]. We identify Cl atoms up to 50Å from the parent molecules. We find that both the radial and azimuthal distributions of Cl atoms depend sensitively on the tunnelling current [3] and that a wide range of surface sites is populated by the (energetic) Cl atoms (probably anions). This behaviour can be explained in terms of an energetic, two-electron dissociation process, as implied by the measured quadratic dependence of the dissociation rate on tunnelling current. We propose a mechanism based on dissociative electron attachment (DA) of the “second” electron to a molecule vibrationally excited by the “first” electron [3]. Such a mechanism explains how one can overcome the symmetry barrier to C-Cl dissociation via electron attachment to the ring states.

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3. P.A. Sloan and R.E. Palmer, submitted.

## Molecular and Supra-Molecular Assembly and Positioning

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One of the key challenges in molecular machines and devices is the reproducible assembly of functional units in an addressable way e.g. in 2D arrays at surfaces. Using a variety of different molecules with specifically designed structure, increasingly complex functional layers have been manufactured and explored. Selective molecular interaction is the generic origin of molecular self assembly [1] and a variety of different mechanisms have been identified: Selective chemical bonding [2], conformational bi-stability [3], and 2D phase behaviour [4] produce distinctly different functional layers. Binary molecular systems which involve longer range dipole forces and entropic mobility provide the basis for an increased periodicity [5]. In conjunction with a conformational mechanism the spacing between individual supramolecular units has very recently been increased to 7.2 nm [6]. Going beyond supra-molecular assembly first *covalent* polymeric networks have been created by a thermally activated chemical reaction [7] and have been used as a template for supra-molecular organisation of ad-C60 molecules. Most recently the first successful assembly of extended molecular layers on insulator thin films has been demonstrated [8]. All these examples have in common that the supra-molecular structures are extremely well defined and identical on a level which is impossible to reach by conventional top-down assembly techniques. Following the discussion of the physics and chemistry involved in the formation of these versatile structures I shall review and update the concept of mechanic and electronic ‘function’ on a single molecular scale.

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- [8] L. Ramoino et al. Manuscript in Preparation

## **Cu(111) surface waves created by the Lander series molecules**

L. Gross, M. Machado, C. Joachim and F. Moresco

Speakers: (1) L. Gross and (2) C. Joachim

Due to scattering of surface state electrons at Lander molecules characteristic standing wave patterns are formed in the vicinity of the molecules, since the Lander extensions are in the same order as the electrons Fermi wavelength. The wave patterns can be used to probe the molecule-metal interface, which is not accessible by STM otherwise. By comparison with calculations the position of the strongest scattering centres inside the molecule can be revealed. Dependence of the standing wave amplitude on the distance between the conjugated board and the metal surface have been calculated using the N-ESQC technique in the perspective of modulating it with an active molecule.

## PROTOTYPES OF ARTIFICIAL MOLECULAR MACHINES AND MOTORS

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The area of nanotechnology is a very broad one. From the chemical viewpoint, nanotechnology can be defined as the marriage between the synthetic talent of chemists with a device driven ingenuity. The chemical, bottom up approach, based on the concepts of supramolecular chemistry, can indeed be very useful to design and construct interesting nanostructures. By using this approach, the macroscopic concepts of a device and a machine can be straightforwardly extended to the molecular level [1]. A *molecular device* can be defined as an assembly of a distinct number of molecular components (that is, a supramolecular system) designed to carry out a complex function, resulting from the cooperation of the simple acts performed by each molecular component. Of particular interest are molecular-scale devices in which the component parts can be set in motion upon appropriate stimulation, that is, *molecular machines* [2].

Molecular machines are ubiquitous in biological systems. Motor proteins are extremely complex assemblies, the structures and detailed working mechanisms of which have been elucidated only in a few cases. Since any attempt to construct *fully artificial* systems of such a complexity by using the bottom-up molecular approach would be hopeless, chemists are trying to construct much simpler nanomachines. In the last few years, synthetic talent, that has always been the most distinctive feature of chemists, combined with a device-driven ingenuity evolved from chemists' attention to functions and reactivity, have led to the design and construction of a great number of very interesting molecular machines and motors [1,2]. Recent examples studied in our laboratories in the solution phase - based on threaded and interlocked molecular systems like pseudorotaxanes, rotaxanes and catenanes - will be presented, including the recently reported molecular elevator [3] and an example of an autonomous linear nanomotor powered by visible light [4]. Performances, limitations and perspectives of this kind of systems will be discussed.

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## **Semiconductor nano-crystals for photon nano-sources**

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Semiconductor Nanocrystals (NCs) have attracted much interest in the past few years due to their unique opto-electronic properties and their possible use for light emitting diodes, photovoltaic cells and biological markers. In the context of molecular nano-machines, semiconductor NCs are expected to play a crucial rôle as photon nano-sources for powering and controlling the operation of complex molecular architectures. As a preliminary step in the fabrication of photon nano-sources, we will present the STM imaging, spectroscopy and manipulation of different kinds (spherical and nanorods) of individual CdSe nanocrystals on atomically resolved surfaces.

## Organic Nanofibers

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Future information technology will be based on nanophotonic devices. In this context the interest in growing and manipulate selectively inorganic or organic nanowires has grown immensely. One very promising class of materials consists of short-chain para-phenylenes (p-nP, n=4-6) which can form semi-conducting films, aggregates or nanofibers with rather delocalised  $\pi$ -electrons. The most important property is that they emit blue light after excitation with either UV light (around 360 nm) or electrons which makes them well-suited candidates for building up active layers in organic light-emitting diodes (OLEDs), organic field effect transistors (OFETs) and other electronic and optoelectronic devices. Depending on the growth conditions oriented needle growth is observed on mica. The growth mechanism of the needles is influenced by strong electric dipole fields on mica which induce a dipole moment in the polarizable organic molecules, leading to an attraction via dipole-induced dipole forces and thus an alignment of the individual organic molecules along the surface dipole orientation. If the molecules possess enough surface mobility (i.e. if the surface is warm enough), aligned, needle-like aggregates of hundreds of  $\mu\text{m}$  can be grown with very well defined molecular orientations and widths between 50-400 nm [1]. Their optical properties are highly anisotropic exhibiting linear waveguiding properties because of their high refractive index. If one increases the intensity of the excitation light, nonlinear optical effects can be observed in the nanofibers [2]. Due to the low photobleaching threshold of the aggregates, femtosecond laser pulses had to be employed as the excitation source. At excitation wavelengths between 770 and 786 nm contributions to the two-photon signal intensity from both two-photon luminescence (TPL) and second harmonic generation (SHG) have been observed, where  $I_{SHG} / I_{TPL} \approx 0.015$ . A  $\chi(2)$  has been obtained which is only half of that for KDP (potassium dihydrogen phosphate), a common material for frequency doubling laser light. Beside details on the nonlinear properties first results on growth of organic nanofibers from functionalized molecules will be reported.

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## **Tracking individual proteins in live cells using semiconductor quantum dots**

Maxime Dahan (Laboratoire Kastler Brossel, ENS, France)

Quantum dots (QDs) are inorganic probes which hold great promises for advanced biological imaging. Because of their small size, brightness and photostability, they offer a favourable compromise between small dyes and large beads for single-molecule experiments, notably in live cells. We used QDs to track tagged-receptors in the membrane of live neurons for durations of tens of minutes. Using standard optical techniques, single receptors can be detected with a high signal to noise ratio (greater than 30) and high spatial resolution (~10 nm), showing that QDs are invaluable tools to study the dynamics of cellular processes at a molecular level.

In this talk, we will discuss the kind of information that can be obtained with single molecule experiments in live cells and what they reveal about the dynamic organization of molecular assemblies. The discussion will be illustrated by experimental data obtained on different biological systems : (i) diffusion domains of glycine receptors in dendrites, (ii) microtubule-dependent directed movements of GABA receptors in growth cones. We will finally indicate future challenges for the use of QDs in cell biology.

## **Functional molecules and transition metal complexes for molecular machines**

Vincent Huc

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91405, Orsay, France

Chemistry provides a huge number of molecular or supramolecular systems exhibiting strong structural fluctuations under various excitations (thermal, electrochemical, photochemical...). But only recently, the possibility to control these fluctuations led to the concept of molecular nanomachines.

During the first part of the lecture, the descriptions of the different strategies currently used to obtain a controlled molecular motion will give us some general features about molecular nanoengines.

Finally, the potential of organometallic catalysis for the realisation of molecular nanoengines will be discussed, and within this frame some future research axes will be suggested.

## How the cell converts energy

Giovanni Cappello

Institut Curie, France

The cells, both for eukaryotic and prokaryotic systems, are thermodynamically unstable. This instability is essentially allowed by two elements: on one hand a membrane isolates the cells from the external world, on the other hand many active proteins transform the energy inside the cell. Molecular motors represent a major family of these proteins: the enzymes catalyse ATP hydrolysis, transforming ATP into the more stable ADP. During the hydrolysis reaction the chemical energy stored in ATP is transformed in mechanical power.

Hundreds molecular motor are involved in cell motility (migration, muscle contraction, hearing...), intracellular transport, organelles dynamics, mitosis and DNA replication and transcription.

The fundamental mechanism of energy conversion, the details of which remain obscure, is the main interest of the physicist. In order to understand this process, it is essential to have access to the dynamical parameter, such the detail of the motion, the force developed by a single molecule and its efficiency.

New experimental techniques, like magnetic tweezers, optical clamps, fluorescence video-microscopy, together with novel theoretical tools, shed light on these questions and permit to propose simple models explaining how the molecular motors function.

The theoretical description, based on single-molecule experiments, can predict the cooperative behavior of many molecular motors. Such behavior is involved in biological relevant phenomenon, like hearing and muscle contraction, and it can be reproduced in in vitro experiments.

**How two-foot molecular motors may walk**

Kazuhiko Kinoshita

*Okazaki Institute for Integrative Bioscience, Japan*

## Nanomanipulation with Laser and STM

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*ORSAY*

Coupling the optical control capabilities of lasers with the ultimate nanoscale spatial resolution of the Scanning Tunneling Microscope (STM) is a long term motivation for operating molecular nanomachines.

I will review various methods combining STM and Laser for the manipulation and the control of nano-object on surfaces. The combination of an excitation by tunnel electrons or photons will be discussed. More specifically, I will illustrate this comparison with the first quantitative results on the photodesorption of hydrogen from Si(100)-(2x1):H assisted by STM. In this study we analyse the surface of Si(100)-(2x1):H before and after irradiation via STM topographies. The laser used is an excimer laser delivering VUV photons at 7.9 eV corresponding to the  $\sigma \rightarrow \sigma^*$  localized transition states of the Si-H bond [1]. An in depth statistic method is used to extract from these observations the average yield of photodesorption of H atoms. Furthermore, the desorption observed induces not only isolated dangling bonds but structural modifications of the surface as well, induced via sub-surface photo-reactions. Previous studies measuring H<sub>2</sub> or H<sup>+</sup> desorbed species by time of flight or STM induce H desorption will be compared [2, 3]. Finally, I will discuss the possibility of inducing photodesorption by VUV light *under* the STM tip.

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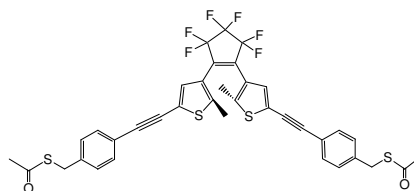
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## Double well unimolecular effect : Photochromism and electrochromism in a molecule

C. Coudret

*CEMES*, France

Molecules such as 1,2-dithienylethene derivatives undergo a reversible photochemical isomerisation process that leads to a dramatic change of their electronic properties. The main consequence is a colour change hence the name of this property (photochromism). In order to use this type reaction to operate a molecular switch, we designed a molecule to be inserted into Self-Assembled Monolayers. The individual behaviour was tested by STM in air by Prof. P. Dumas (Marseille) and his collaborators and revealed an unexpected blinking process.



Molecule for Self-Assembled Monomayer studies

This prompted us to explore the electrochemical behaviour of this molecular unit. A family of representative compounds was then prepared, and once oxidized, all show (at least for one of their photoisomers) an irreversible reactivity. In most of the cases, the reaction was clearly identified to exactly parallel one of the photochemical path. Thus an electrochromic behaviour has been detected for all these compounds. The lecture will presents synthetic data as well as results from STM, electrochemistry and theoretical calculations .

## **Ordering and dynamics for a family of oligo(phenylene ethynylene)s on Au(111) studied by UHV-STM.**

T. R. Linderoth, C. Busse, S. Terkelsen, L. Petersen, M. Nielsen, K.V. Gothelf, and F. Besenbacher

To realize the goal of functional structures formed by molecular self-assembly, systematic studies of factors directing the assembly process are required. Using UHV-STM we have performed a comparative study of adsorption structures formed by a family of organic molecules (oligo(phenylene ethynylene)s) on the Au(111) surface. By systematically varying the molecular geometry, the adsorption motif can be changed from parallel to upright, and by varying the molecular interaction chemistry, the importance of intermolecular hydrogen bonding on the formed structures can be assessed. Many of the investigated structures are chiral and we find there is a high correlation between the molecular tiling patterns and the surface conformers assumed by the adsorbed molecules. The correlation is enabled by a surprising intramolecular switching mechanism allowing the adsorbed molecules to flip between different surface conformers. Activation barrier and prefactor for this dynamic intramolecular process is determined from time-resolved STM data. Finally, ongoing experiments regarding intermolecular covalent cross-linking and metal complexation are touched upon.

## **Scanning Probe Energy Loss Spectroscopy**

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Scanning Probe Energy Loss Spectroscopy (SPELS) is a new technique that can be viewed as a hybrid between scanning tunneling microscopy (STM) and electron energy loss spectroscopy (EELS). The fundamental advantage of SPELS is the ability to provide local EELS data from a surface. A tungsten STM tip in field emission mode is used as a local source of electrons, with a tip bias between 50V and 150V. The process of field emission gives an associated energy resolution of  $\sim 300\text{meV}$ . This allows us access to plasmon excitations, molecular electronic excitations and interband transitions. In this presentation we will discuss the SPELS spectra of a graphite surface as well as the instrument's ability to detect local secondary electron emission. We shall also provide evidence of local spectroscopic features in SPELS, that reinforces our main goal of spectrally characterizing size selected metallic nanoclusters.

## Single molecule mechanics of myosin motors using optical tweezers

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The invention of 'optical tweezers', the single beam gradient-force optical trap, has brought about a revolution in molecular cell biology and physiology, which made it possible to study the physical properties of macromolecules at the single molecule level. Using optical tweezers and related optical technology, one can apply piconewton sized loads and measure nanometre-level displacements. Forces and displacements of this magnitude are typical of the so-called motor-proteins, responsible for generating biological movement. In this talk results from recent single molecule studies of the motor protein myosin will be discussed, along with aspects of instrumentation and analysis that make such studies possible.

## Controlling the Dynamics of a Single Atom in Lateral Atom Manipulation\*

Joseph A. Stroscio and Robert J. Celotta

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The ability to manipulate single atoms with the scanning tunneling microscope (STM) stirs one's imagination because of the vast opportunities made possible for building atomic scale devices and nanostructures. Understanding the host of interactions in the STM tunnel junction, and their optimization, is required for efficient and reliable atom manipulation needed for large-scale autonomous assembly of atomic devices.

In this talk I will discuss our work on using atom manipulation imaging and the noise characteristics of the tunneling current as probes of the physics of the atom manipulation process [1]. I will first discuss the dynamics of the Co atom in the context of a manipulated atom image, which is obtained by scanning a single Co atom across the Cu(111) surface with the Co atom trapped in the tip induced potential well. This image (see Fig. 1) reveals the binding sites of the substrate and the variation in the potential energy surface for Co on Cu(111). When the Co atom is positioned over the hcp site, dynamic behavior is observed both in the manipulated atom image and in the tunnel current. This site dependent noise in the tunneling current is in the audio range and can be heard as the atom is dragged over the surface. This dynamic behavior corresponds to the Co atom switching between the neighboring (and almost equivalent) fcc and hcp sites of the Cu(111) surface. This occurs by the creation of an ideal, tunable, multi-well potential by the tip-atom interaction. An ideal double well potential is created by positioning the probe tip slightly off center from the hcp site. Two-state transfer rates between the hcp and fcc sites are obtained by measuring the distribution of residence times in each state. The transfer rates show two distinct regimes. A transfer rate independent of tunneling current, voltage and temperature that is ascribed to quantum tunneling between the two wells, followed by a transfer rate with a strong power law dependence on current or voltage, indicative of vibrational heating by inelastic electron scattering.

\* This work is supported in part by the office of Naval Research.

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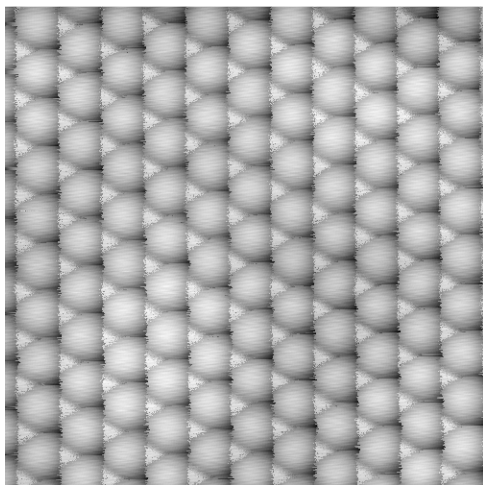


Figure 1: Manipulated atom image, 2.5 nm x 2.5 nm, of Co on Cu(111) obtained by scanning a single Co atom over the Cu(111) surface. Tunnel current 50 nA, sample bias – 5 mV, T = 4.3 K.

## **The IBM Nanostencil: Design and first experiments**

P. Zahl

IBM Zurich Research Laboratory

The nanostencil is a novel tool for resistless lithography. It allows the direct patterning of complex nanometer-sized structures composed of a wide range of materials in a UHV environment. This is combined with state-of-the-art scanning probe microscopy techniques (AFM, STM) and an electronic 4-point probe. Moreover, all these capabilities are in-situ and auto-aligned in the field of view. The direct patterning is based on the shadow-mask technique and allows multi-mask processes in a static and dynamic manner.

## Dynamics and self-assembly of organic adsorbates on single-crystal metal surfaces

Roberto Otero, Maya Schöck & Flemming Besenbacher

The adsorption and self-assembly of organic molecules on single-crystal surfaces has attracted much attention lately due to its potential applications in fields ranging from molecular electronics to biocompatible interfaces. The supramolecular structures formed upon deposition of molecular species on solid surfaces depend upon the molecular architecture and the distribution of functional groups on one hand, which determines the thermodynamically stable molecular arrangement, and on the other hand on kinetic factors like thermal diffusion, spontaneous rotations and conformational dynamics. In this talk we will describe different experiments designed to shed light on both aspects of the physics of adsorbed organic species on solid surfaces. In particular we will address the following issues:

1. Coupling between linear diffusion and the rotational degree of freedom for adsorbed “violet lander” (VL) molecules: Local-and-key mechanism in diffusion
2. Conformational dynamics of adsorbed VL molecules: role of diffusing adatoms?
3. Self-assembly of guanine quartets on Au(111): cooperative hydrogen bonds.
4. Molecular recognition in binary mixtures of DNA bases on Au(111)

## Assembly of chemical modules under physical constraints : a road to engineer biological complexity ?

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Several mathematic models were proposed around 1970 to account for “complex” biological behaviors [1]. Bistability, oscillations, chaos do emerge from their dynamic properties. Unfortunately, these macroscopic models do not correspond to any kinetic law that can be currently observed in chemistry ; the Belousov-Zhabotinsky reaction remains singular. In fact, chemists have no key to design the microscopic units (molecules and chemical reactions) giving rise to such dynamic behaviors. This is especially frustrating in organic chemistry that governs metabolisms of living beings.

Our group addresses molecular engineering of complex behaviors in another way : we design classes of molecular structures and of “classical” chemical reactions that provide complex behavior after a mechanistic reduction [2] that implies appropriate values of rate constants under external constraints (reservoirs of reactants, external potentials,...). In our approach, macroscopic complexity is solved at lower scales of description.

Two major conclusions emerge from our theoretical analyses [3] : i) a small number of specific microscopic processes is sufficient to reproduce several complex behaviors ; ii) control over chemical kinetics is essential to engineer complex phenomena : rate constants must be contained in narrow domains. After an overview of our theoretical frame, this lecture will list some chemical challenges to be addressed to afford the most promising complex behaviors.

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## **Changing the conformation of single molecules by manipulation with the STM tip**

L. Grill, F. Moresco, K.-H. Rieder, S. Stojkovic, C. Joachim

The deposition of Lander molecules onto Cu(110) at room temperature leads to a particular adsorption configuration where the central board of the molecule is located on a metallic nanostructure. This system enables a rotation of the molecular legs without a translation of the entire molecule. Manipulation of these molecules, i.e. a controlled change of their intramolecular conformation, with the STM tip is studied. Attractive and repulsive forces are used in the case of lateral manipulation, where the STM tip is moved laterally across the molecule. In the case of the so-called vertical approach manipulation, only attractive forces are responsible for the conformational change. The dependence of this manipulation process on the bias voltage and the lateral and vertical tip position is discussed by means of the underlying interaction between the STM tip and the molecule.