

ESF – Science Meeting – Final Report

Conference / Winter School

« Addressing, Transport and Storage of information by single atoms and molecules »

Les Houches, January 13 – 18, 2013

A) Summary

This meeting was organised by the members and with the support of the European FET-OPEN project ARTIST (Alternative Routes Towards Information Storage and Transport at the atomic and molecular scale), www.artist.cemes.fr.

The fields of molecular scale electronics and molecular machines are currently very active because of their long term potential and the fast approaching limits of the conventional top-down lithography-based large scale integration. The expected advantages of these bottom-up approaches are now well-known: ultimate size, processing, cost, possibility to design finely-tuned molecular devices, self-assembly, scalability and energy consumption.

But despite thousands of publications and some spectacular breakthroughs on single molecular devices (mostly by scanning probe experiments on metallic surfaces or in break-junction experiments) or large ensembles of molecules in solution (by electrochemistry or optics), all these devices are isolated, thus lack intermolecular communication, even though this is the key prerequisite for applications. Classical electrical circuitry by metallic wiring cannot be used at this scale for several reasons (size, reproducibility, stability, complexity of fabrication); electron transport by molecular wires is so far limited by the electrode-molecules contact resistances, as well as small and exponentially decreasing conductances. Therefore, a complete paradigm shift is required to explore new single electron and proton technologies coupled to optical and/or electrical addressing for information transport and storage at the nanoscale.

Recent developments have shown that it is now possible to tackle these ambitious objectives at the single atom or molecule level, on films of insulators, bulk insulators, or wide band-gap semi-conductors by: a) **non-contact addressing by nano-optics, in particular plasmonics** and by electrostatics, b) **long distance information transport by intramolecular single electron transfer, plasmon mediated intermolecular energy transfer, and intermolecular propagation of proton transfer or by conformation transfer**, c) **information storage in conformations, or by charge trapping in atoms and molecules**.

The objectives of this workshop were:

- 1) to bring scientists from surface science and nanoscale optics / plasmonics together, and to discuss mutual opportunities and benefits from different techniques and approaches
- 2) to foster students and post-docs towards this multidisciplinary approach (chemistry, simulation and theory, nano-optics, scanning probe microscopies).

B) Scientific content of and discussions at the event

While advanced fabrication and characterization enables optical methods to probe deeper into the nanoscale, supramolecular approaches can nowadays build larger and more complex molecular structures. It is thus conceivable that when structure dimensions approach each other novel exciting possibilities for fundamental research on the ultimate limits of addressing, transporting and storing « information » (optical or electronic excitations, conformations, charge, ...) emerge. It was before this background that scientists (including a large share of Ph.D. students and young postdocs) met to discuss novel concepts and ideas to

extend and combine their respective fields, i.e., nano-optics / plasmonics and molecular electronics, with a strong emphasis on scanning probe techniques.

One such approach that has proven successful recently is the excitation of plasmons in metal nanostructures by a scanning tunneling microscope, a topic that opened the conference with presentations from Orsay and Graz. The reach and limitations of plasmonic modes for addressing nanoscale volumes was further emphasized in contributions from Hefei, China and Dijon and in vivid discussions on how atom-scale surface science techniques can be brought together with experimental optical methods.

The current state of the art in scanning probe technique was introduced in the talks from IBM Rüsclikon, Aalto, Berlin, Basel, Argonne National Lab and others. The unprecedented resolution shown recently in scanning force microscopy opens new venues in the imaging of molecules, while scanning probe manipulation can now tackle the building of larger molecular architectures. Here, on one hand theory and simulation talks from Toulouse, Liverpool, Montreal and others provided important explanations of the underlying physics and chemistry, and additional aspects and perspective. On the other hand, chemical synthesis provides the starting point for virtually all of this research, and contributions from Toulouse intensively discussed this point.

Overall, the discussions at the event strongly benefited from the combination of a core group formed by the ARTIST project members that work on combining the realms of scanning probe / surface science with nano-optical / plasmonic methods for three years now, with international attendees providing new insight and perspectives.

C) Results and impact of the event on the future directions of the field

As the ARTIST project is coming to an end in summer 2013, there was a focus on new cooperations and projects. Clearly, the excitation of plasmon modes by tunneling electrons shall be further explored, as this field (although based on effects known for a long time) could make significant advances towards bridging the gap between the electronic and the optical scales, when exploiting recent experimental and theoretical progress. Novel molecular architectures with built-in electrical, mechanical or optical functionalities will be further pursued, and scanning probe techniques are to be expected to further extend their range, besides functionalized tips being established as high-resolution standards. Overall, it was agreed upon that the interdisciplinary cooperation of people from physics and chemistry is indispensable to push the field further, and that this shall include technical developments to combine surface science with nano-optical methods.

ARTIST Winter Workshop
Addressing, Transport and Storage
of information
by single atoms and molecules

January 13-18th, 2013

Les Houches, France

Program

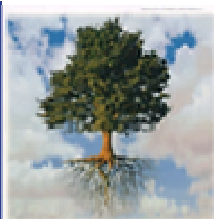
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Program

Sunday, January 13th, 2013

19:15 - 19:30 Opening address

André GOURDON (Cemes, Toulouse, France)

19:30 – 20:45 Dinner

Monday, January 14th, 2013

SESSION 1

8:30 – 9:15 Probing plasmon modes with photons and electrons

Joachim KRENN (Univ. Graz, Austria)

9:15 – 9:45 Synthesis of a donor-acceptor porphyrinate rotor mounted on a naphthalocyanine stator

Roman STEFAK (Cemes, Toulouse, France)

9:45 - 10:15 Electrical excitation of surface plasmons on gold nanowires with scanning tunnelling microscope

Benoît ROGEZ (Ismo, Orsay, France)

10:15 – 10:30 Coffee break

SESSION 2

10:45 – 11:30 Scanning probe microscopy of single molecules on insulating films: Orbital imaging, molecular geometry and intramolecular charge distribution

Gerhard MEYER (IBM Res. - Zurich, Rüschlikon, Switzerland)

11:30 – 12:15 Plasmonic Purcell factor: control and addressing of optical nanosources

Gérard COLAS des FRANCS (ICB, Dijon, France)

12:30 - 19:00 Lunch and afternoon break

19:00 - 19:30 Welcome drink

19:30 - 20:45 Dinner

SESSION 3

20:45 – 21:15 A redox molecular switch on an ultra-thin polar film: a density functional study

John SHARP (SSRC/Dep. Chem., Univ. Liverpool, UK)

21:15 – 22:00 Conformational molecular switch and controlled rotational motion of azobenzene and azobenzene derivative molecules

Young KUK (Dep. Phys. Astron., Seoul Nat. Univ., Korea)

Tuesday, January 15th, 2013

SESSION 4

8:30 – 9:15 Single molecular plasmonics at the nanoscale

Zhenchao DONG (Hefei Nat. Lab. Phys. Sci. Microscale, Anhui, PRC)

9:15 – 9:45 Advanced analysis of calculated scanning probe microscopy images for conformational and structural determination of various molecule/surface systems

Xavier BOUJU (Cemes, Toulouse, France)

9:45 - 10:15 Ultrafast hot electron emission from plasmonic nanoparticles
Andreas TRÜGLER (Inst. Phys., Univ. Graz, Austria)

10:15 – 10:30 Coffee break

SESSION 5

10:30 – 11:15 Scanning probe microscopy experiments on atomically well-defined graphene nanostructures

Peter LILJEROTH (Dep. Appl. Phys., Aalto Univ., Finland)

11:15 – 11:45 Investigating assemblies of domino molecules on a (111) gold surface

Wojciech GREŃ (Cemes, Toulouse, France)

11:45 – 12:30 Influence of alkali halides crystals on the growth of molecular layers

Laurent NONY (IM2NP, Aix-Marseille Univ. France)

12:30 - 19:30 Lunch and afternoon break

19:30 - 20:45 Dinner

Wednesday, January 16th, 2013

SESSION 7

8:30 – 9:15 Charging and conformation changes in Cu(dbm)₂

Sébastien GAUTHIER (Cemes, Toulouse, France)

9:15 – 9:45 Dynamics of charging and bond formation of adsorbates on an ultrathin, insulating film supported by a metal substrate: a density functional theory study based on a perfect conductor model

Ivan SCIVETTI (SSRC, Univ. Liverpool, UK)

9:45 - 10:15 Bond-order discrimination by atomic force microscopy

Bruno SCHULER (IBM Res. Zurich, Rüschlikon, Switzerland)

10:15 – 10:30 Coffee break

SESSION 8

10:30 – 11:15 Frontiers of STM manipulations: imaging atomic spin to operating nanomachines

Saw Wai HLA (Argonne Nat. Lab., Ohio Univ., USA)

11:15 – 11:45 Controlled coupling of single photon emitters to metallic nanowires

Christian GRUBER (Inst. Phys., Univ. Graz, Austria)

11:45 – 12:30 Imaging and directed rotation of single molecules by non-contact force microscopy

Ernst MEYER (Dep. Physics, Univ. Basel, Switzerland)

12:30 - 19:30 Lunch and afternoon break

19:30 - 20:45 Dinner

SESSION 9

20:45 – 21:30 Towards fast, efficient and accurate electronic structure of insulator-metal interfaces

Matt WATKINS (Dep. Phys. & Astron., UCL, London, UK)

21:15 – 22:00 Spin-polarized transport in Mn-based systems

Maria SORIANO (Autonom. Univ. Madrid, Spain)

Thursday, January 17th, 2013

SESSION 10

8:30 – 9:15 Computing toward the reverse problem in STM imaging

Alain ROCHEFORT (Polytechnique Montréal, Canada)

9:15 – 9:45 Towards SWAP single molecule – A chemical approach

Jacques BONVOISIN (Cemes, Toulouse, France)

9:45 - 10:15 A nonlocal approach to atomic manipulation
Duncan LOCK (Univ. Bath, UK))
10:15 – 10:30 Coffee break

SESSION 11

10:30 – 11:15 Bottom-up assembly of molecular chains and their manipulation by STM
Alex SAYWELL (Fritz-Haber-Inst., Berlin, Germany)
11:15 – 11:45 Controlling spins in adsorbed transition metal complexes by on-surface magnetochemistry
Christian WÄCKERLIN (Paul Scherrer Inst., Villigen, Switzerland)
11:45 – 12:30 On-surface synthesis and characterization of conjugated poly-phenyl systems
Nian LIN (Dep. Physics, Hong Kong Univ. Sci. Technol., Hong Kong)
12:30 - 19:30 Lunch and afternoon break
19:30 - 21:45 Conference dinner: Alps

Friday, January 18th, 2013

SESSION 12

8:30 – 9:00 Low temperature UHV-STM investigations of Ruthenium complexes: progresses towards a SWAP mono-molecular logic gate
Loranne VERNISSE (Cemes, Toulouse, France)
9:00 – 9:45 Switching porphyrin derivatives on Au(111)
Johannes MIELKE (Fritz-Haber-Inst., Berlin, Germany)
9:45 – 10:15 Adsorption, mobility, and growth of Co-Salen molecules on bulk insulators
David GAO (Dep. Phys. & Astron., UCL, London, UK)
10:15 – 10:30 Coffee break

SESSION 13

10:30 – 11:15 Using the scanning tunneling microscope to excite localized and propagating surface plasmons: light from electrons
Elisabeth BOER-DUCHEMIN (Ismo, Orsay, France)
11:15 – 11:45 Molecular states of trinaphthylene molecules on hydrogen passivated Ge(001) surface
Marek KOLMER (Dep. Phys. Nanostruct. Nanotech., Jagiellonian Univ., Krakow, Poland)
11:45 – 12:00 Concluding remarks
André GOURDON (Cemes, Toulouse, France)
12:30 Lunch and departure

Posters

- 1- Charge distribution and Scanning Tunneling Spectroscopy of CuPC analyzed by tuning-fork AFM/STM
S. Fremy (Dep. Physics, Univ. Basel, Switzerland)
- 2 - Scanning probe microscopy and spectroscopy of nanodiamonds under illumination.
Rémy Pawlak (Dep. Physics, Univ. Basel, Switzerland)
- 3- Laser fields at flat interfaces: plasmon resonances of aluminium and silver low index surfaces
Georges Raseev (Ismo, Orsay, France)