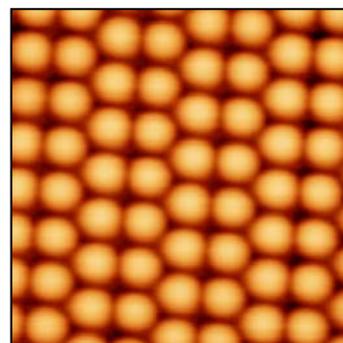
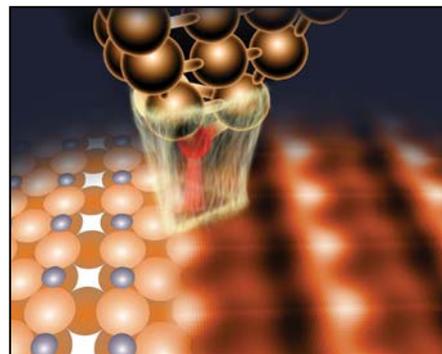
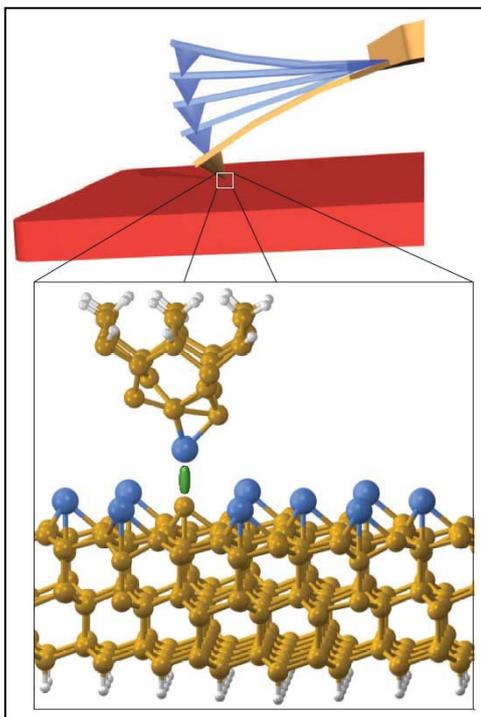


XXI International Summer School "Nicolás Cabrera"  
**NEW FRONTIERS IN SCANNING FORCE MICROSCOPY: FROM  
 ULTRAHIGH-VACUUM TO BIOLOGICAL MATERIAL**

14 - 18 July, 2014

Residencia "La Cristalera"  
 Miraflores de la Sierra  
 Madrid - Spain



With the collaboration of:

**Fundación BBVA**





## XXI International Summer School "Nicolás Cabrera"

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### *Prof. Nicolás Cabrera*



For those of us who had the pleasure of knowing him in his mature years, Nicolás Cabrera comes as close as humanly possible to the ideal figure of a renowned scientist and a perfect gentleman, someone who has a keen insight in the ways of nature and at the same time is fully at ease with his fellow humans, always benevolent and encouraging, yet also reserved and detached in his judgment. Science and academics were in his family line, as he was the son of Blas Cabrera, the leading physicist in Spain between the two world wars. He was given by birth the opportunity to study and work with famous people in France and England, and happily his natural talent was up to the challenge and thrived on it. But he also knew sorrow in his life as an exile from a country torn by civil strife. In his years in North America, there was always an undertone of sadness in his eyes and a longing to return to a free and democratic Spain.

Jack Mitchell recalls that the Cabrerases were living in an apartment in Paris when he recruited Nicolás to come to Bristol and work with Neville Mott as a post-doc. In Bristol he produced not only the fundamental theory of crystal growth, but also, with Mott, an important paper on the theory of the oxidation of metals [1]. It was perhaps this work that most impressed Allan Gwathmey of the Chemistry Department at the University of Virginia, and led him to arrange with Jesse Beams, then Chairman of Physics, to offer Cabrera a position, which he accepted in 1952. His scientific and leadership impact at Virginia extended also to Materials Science and other areas of Engineering, as he actively pursued interdisciplinary contacts, and his work transcended narrow boundaries.

My personal recollections of Cabrera date from a splendid spring day in 1962, when I came to give a seminar on dislocation dynamics at the University of Virginia. Those were the happy days in which young physicists did not have to apply for jobs, and I was barely aware of the fact that this was, in effect, an interview. Cabrera, who had just become Chairman, took a genuine interest in what I was doing, asked penetrating questions, and at the same time made me feel completely at ease, no small feat considering that I knew he was an author of the Burton-Cabrera-Frank theory of crystal growth [2], which was already enshrined in textbooks then (and appears even more fundamental today, more than fifty years later). Cabrera was a very effective recruiter at

all levels, making effortless use of his natural charm and cultivated European style in personal contacts, and keeping a high awareness of possible candidates through his high-level contacts in the scientific world. Four years later, when I arrived in Charlottesville as the newest faculty member, Cabrera himself came to meet us at the station, which impressed my wife no end.

With Jack Mitchell, Doris Wilsdorf and her husband Heinz (in Materials Science) Virginia was then a leading center of research on dislocations and mechanical properties. Cabrera, however, was always looking for fresh fields. When he called me to his office to tell me of problems he had in mind, I was surprised (but should not have been) that it had nothing to do with crystal growth or dislocations. Instead, he told me of experiments under way in Aerospace Engineering on atom-surface interactions. He thought that atom scattering could be used to detect surface phonons, analogously to neutron scattering in the bulk. The kinematics was right but some approximate cross sections had to be computed to prove that the method was feasible. It sounded complicated enough that we needed a graduate student to help, and as it happened Dick Manson had just asked me for a thesis project. After we read up on scattering theory and surface elastic waves, everything turned out pretty much as Cabrera had anticipated for a simple elastic hard wall [3]. Actual surfaces are much more complicated, as we learned from Frank Goodman, who was working with the Aerospace people. The four of us hammered out a long paper [4], which required some effort to develop a common language, coming as we did from different specialties. Cabrera kept us together, focussing on the physics, and we deferred to him, naturally. This is something I have seen happen repeatedly in collaborations with him. He was a good listener and a natural leader; he did not dominate a discussion but came to the essential point, noting quickly where there was a real disagreement and where it was just a matter of semantics.

In 1967 Cabrera went on leave for a year in Caracas, and then accepted a leadership post at the resurgent Autonomous University of Madrid when Franco was still in power. There were several reasons for these developments. The Physics Department at Virginia had grown and prospered under Cabrera's leadership, not only in Solid State, but also in Nuclear Physics. Unfortunately, some of the senior people had strong and apparently incompatible personalities, although they all had good relations with Cabrera. His patience and diplomatic skills were taxed, especially after some petty problems developed over the management of the nuclear facilities. Scheming and pettiness were so alien to his nature that he was saddened by them, and also felt that he had better ways to spend his time and energy. Although the Cabrera children had grown up as Americans and Blas, then enrolled at Virginia, was clearly on his way to his own physics career in the U.S., nostalgia for Spain was always near the surface, especially for Nicolás's lively wife, Carmen. There were evenings at the Cabrerias with singing and guitars, and as the party took wing more and more of the songs were Spanish. But fundamentally it was Nicolás who felt an obligation to return to Spain and rebuild science there.

That it took courage and dedication to do so was apparent to me at the Varenna Summer School on 'Dynamic Aspects of Surface Physics' in 1974, organized and directed by Frank Goodman. Although several aspects of surface physics were covered at this school, it was a seminal event in the field of atom-surface interactions, with Boato and Cantini reporting their high-quality diffraction data, Giorgio Benedek lecturing on surface phonons, and J.P. Toennies as one of the 'students' absorbing it all and preparing to make the study of surface phonons by He scattering a reality in his laboratory. Cabrera was expected to be one of the main lecturers, but he was able to attend only part of the time, as the situation in Spain had taken a turn for the worse. Incidentally, he was accompanied by Javier Solana, who was then his assistant in Madrid, before embarking on his still-rising political career. (He had come to Virginia to complete his graduate studies shortly before Cabrera left).

Things were dramatically different in 1980, when I was Cabrera's guest at the Autonomous University of Madrid, in the Institute that now bears his name. He was now Don Nicolás, an almost legendary figure to the young generation of physicists in his own country. Those were heady days for Spain and its reborn democracy. Cabrera's dreams and hopes had come true, and yet he was still striving for improvement, trying to set up his institution in a new, less bureaucratic way. In the midst of all the political excitement and the administrative struggles, he still found time to take out a yellow notepad, legal size, and work out equations and ideas.

Nicolás Cabrera was not driven by ambition or the hunger for recognition; after recognition and power came to him, he was as gentle and considerate as before. He knew adversity and acknowledged that the world is far from perfect, but remained an incurable optimist and was simply convinced that if one does the right thing it will all work out. And in the end it did.

V. Celli

Department of Physics,

University of Virginia

[1] Cabrera N and Mott N F 1999 Rep. Prog. Phys. 12 163

[2] Burton W C, Cabrera N and Frank F C 1951 Trans. Roy. Soc. (London) A243 299

[3] Cabrera N, Celli V and Manson R 1969 Phys. Rev. Letters 22 346

[4] Cabrera N, Celli V, Goodman F O and Manson R 1970 Surf. Sci. 19 67

*This text can be found in the web page of the Nicolás Cabrera Institute ([www.uam.es/inc](http://www.uam.es/inc)). It was written on the occasion of a homage to Prof. Nicolás Cabrera (1913-1989), and published in Journal of Physics Condensed Matter, Volume 14, Issue 24 (2002).*

Nicolás Cabrera was an outstanding scientist who strongly influenced the development of Physics in Spain in the last third of the twentieth century. His personal contributions to science are widely known and cited today. As the current head of the Department of Condensed Matter Physics, in the Universidad Autónoma de Madrid, I will refer briefly to his role in the creation of the Physics Department of our University.

As with many other Spanish scientists, writers and artists, Cabrera was exiled as a consequence of the civil war. Before this, the new physics developed mainly in Europe had also permeated Spanish society. This led talented young people to go abroad to learn in the most prestigious laboratories. One of the most prominent of these was Nicolás's father, Blas Cabrera, who was then the leading Spanish figure in the growing international activity on physics. He was the head of a modern and well equipped laboratory of physics and chemistry, close to the students' residence where Dalí, García-Lorca and Buñuel were living then. He made an important experimental contribution to magnetism, and it was on this subject that Nicolás Cabrera performed his first experiments under the supervision of S Velayos.

At that time, scientists such as Santiago Ramón y Cajal, Blas Cabrera and others contributed, through their talent and efforts, to a small 'golden age' of Spanish science. Civil war swept away all this blossoming activity. More than thirty years later, Nicolás often dreamt of emulating his father's endeavours for the development of science in Spain.

The opportunity came in the 1960s when he accepted the offer of the Spanish Minister of Education, Villar Palasí to set up the Department of Physics of the new Universidad Autónoma de Madrid. In this he encouraged Cabrera to adopt the same criteria of quality and efficiency that he had used as head of a new department in the University of Virginia. For many young people beginning their careers in physics then, myself included, Cabrera was a mythical figure. His return to Spain with the aim of forming a new and modern Department of Physics was very exciting for us, and we wanted to be part of it. His great talent and personal qualities enabled him to quickly assemble an excellent group of young scientists. He was granted autonomy by the authorities to offer positions according to his personal criteria, fulfilled by considering mainly CVs, recommendation letters and interviews.

The early years were extremely exciting due to the friendly and creative atmosphere promoted by Cabrera. Many reputable scientists visited our Department and gave interesting seminars, so valued by Cabrera as to make attendance quasi-compulsory. It is impossible in a short space to give a full account of all the innovations that he introduced in teaching and research; we felt that our department was creative and competitive, and our scientific standards were soon recognized by the international community.

Although Cabrera dedicated much time to organizational work, he made a great effort to continue the investigations on surface physics previously undertaken in Virginia. An ambitious plan was launched, following his arrival to Madrid, to build a machine to perform experiments on atomic-beam scattering by surfaces. That became the most important experimental challenge of this period. Former colleagues on surface physics, such as Vittorio Celli, spent prolonged periods in our department working in Cabrera's research group. Unfortunately all these exciting activities suffered the suppressions of the University governors and the Ministry of Education during Franco's last years. Several professors were banned from the university for their political opinions. Others, who came to Spain attracted by Cabrera's project, had to leave the country due to the hostile atmosphere created by the political authorities. It was very sad for us to realize that such attitudes found support among many representing the Spanish academic establishment.

Cabrera's work stood out among the extremely low scientific level of most of the university departments and research centers of physics in Spain at that time. Fortunately, this devastating period concluded with Franco's death, and Cabrera's projects survived. During this dark time Cabrera thought often of going back to the USA, but he stayed, out of consideration for the young people that he had engaged on his personal challenge. He had the opportunity to see his work bear fruit, and that the steps he had taken became an irreversible turning point in the development of physics in Spain.

S Vieira

Department of Condensed Matter Physics,

Universidad Autónoma de Madrid

*This text can be found in the web page of the Nicolás Cabrera Institute ([www.uam.es/inc](http://www.uam.es/inc)). It was written on the occasion of a homage to Prof. Nicolás Cabrera (1913-1989), and published in *Journal of Physics Condensed Matter*, Volume 14, Issue 24 (2002).*



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### *Introduction*

#### *School scope and goals*

Since its invention in 1986, Force Microscopy has become a fundamental tool for studying materials properties at the atomic scale. Due to its high spatial resolution and its ability to manipulate atomic objects, it has contributed in a great extent to the development of Nanoscience and to the study of biological processes. In the last few years, new dynamic force microscopy techniques have achieved atomic or molecular resolution in a broad range of materials from magnetic systems in ultra-high vacuum to proteins and DNA in vitro.

These techniques are able to provide atomic-scale information on both the structure and the mechanical and electrical properties of these material, including subtle changes in charge distribution associated to interatomic bonding, with an unprecedented detail. Among the recent examples, AFM has made it possible to visualize in real space, for the first time, different chemical bonds, including strong covalent intramolecular ones, hydrogen bonding and metal coordination bonds; and to obtain the structure of a molecule with potential clinical applications where traditional chemistry techniques have failed.

The goal of the Summer School is to provide a comprehensive view of the most recent experimental advances in force microscopy, from cryogenic and ultra-high vacuum environments to the physiological conditions necessary for the study of biological materials, as well as on the latest theoretical developments towards the interpretation of these experiments. With that purpose, we have invited the world scientific leaders in the field of force microscopy.

#### *School Topics*

- New advances in experimental scanning force microscopy
- Single molecule applications in liquids: DNA packing, virus assembly, etc...
- High resolution imaging with scanning force microscopy under UHV or liquids
- Simultaneous scanning force/scanning tunneling microscopy
- Theory in scanning force microscopy

#### *Organizers*

##### **Rubén Pérez**

Dpto. de Física Teór. de la Materia Condensada  
Facultad de Ciencias  
Universidad Autónoma de Madrid  
[ruben.perez@uam.es](mailto:ruben.perez@uam.es)

##### **José María Gómez-Rodríguez**

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[josem.gomez@uam.es](mailto:josem.gomez@uam.es)

## **INVITED SPEAKERS**

**Michael Crommie** University of California, Berkeley (USA). Pages 20, 46, 47

**Óscar Custance** National Institute for Materials Science, Tsukuba (Japan). Pages 21, 40

**Adam Foster** Aalto University, Helsinki (Finland). Pages 22, 42

**Takeshi Fukuma** Frontier Science Organization Kanazawa University, Kanazawa (Japan). Pages 23, 43

**Ricardo García** Instituto de Ciencia de Materiales de Madrid, CSIC, Madrid (Spain). Pages 24, 49

**Franz Giessibl** University of Regensburg (Germany). Pages 25, 38

**Leo Gross** IBM Zurich Research Laboratory, Rüschlikon (Switzerland).Pg.26, 45

**Peter Grutter** McGill University, Montréal (Canada). Pages 27, 48

**Suzanne Jarvis** Conway Institute of Biomolecular Research, University College, Dublin (Ireland). Pages 28, 39

**Stephen Jesse** Center for Nanophase Materials Sciences, Oak Ridge National Laboratory (USA). Pages 29, 50

**Ernst Meyer** University of Basel (Switzerland). Pages 30, 55

**José Ignacio Pascual** Nanoimaging (CIC9), CIC Nanogune Donostia– San Sebastian (Spain). Pages 31, 51

**Alexander Schwarz** Institute of Applied Physics and Interdisciplinary Nanoscience Center, University of Hamburg (Germany). Pages 32, 41

**Udo Schwarz** School of Engineering and Applied Science, Yale University, New Haven (USA). Pages 33, 52

**Hirofumi Yamada** Kyoto University, Kyoto (Japan). Pages 34, 44

## **INVITED CONTRIBUTIONS**

**Agustina Asenjo** ICMN-CSIC, Madrid (Spain). Pages 35, 54

**Pedro J. de Pablo** Universidad Autónoma de Madrid (Spain). Pages 36, 53

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# Scientific Program

Sunday 13 July 2014

17:00-20:00	Registration and check-in
21:00	Dinner

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Monday 14 July 2014

## Morning Session Day 1

Session Chair *José María Gómez-Rodríguez (Universidad Autónoma de Madrid, Spain)*

8:30-9:00 Opening

9:00-9:50 *Atomic force microscopy at the pico scale. (Part I)*  
**Franz Giessibl** University of Regensburg (Germany)  
Invited speaker. Page 38

9:50-10:40 *Unraveling nature's secrets with AFM (Part I)*  
**Suzanne Jarvis** Conway Institute of Biomolecular Research, University College, Dublin (Ireland)  
Invited speaker. Page 39

10:40-11:20 Coffee break

11:20-12:10 *Atom manipulation, single-atom chemical identification and sub-molecular resolution by silicon-cantilever based AFM (Part I)*  
**Óscar Custance** National Institute for Materials Science, Tsukuba (Japan)  
Invited speaker. Page 40

12:10-13:00 *Magnetic Sensitive Force Microscopy (Part I)*  
**Alexander Schwarz** Institute of Applied Physics and Interdisciplinary Nanoscience Center, University of Hamburg (Germany)  
Invited speaker. Page 41

13:00-15:00 Lunch

## Afternoon Session Day 1

Session Chair *Rubén Pérez (Universidad Autónoma de Madrid, Spain)*

15:00-15:50 *Atomic force microscopy at the pico scale. (Part II)*  
**Franz Giessibl** University of Regensburg (Germany)  
Invited speaker. Page 38

15:50-16:40 *Simulating Atomic Force Microscopy: (I) Introduction to modern computational approaches*  
**Adam Foster** Aalto University, Helsinki (Finland)  
Invited speaker. Page 42

16:40-17:10 Coffee break

17:10-18:00 *Instrumentation and applications of liquid-environment FM-AFM (Part I)*  
**Takeshi Fukuma** Frontier Science Organization Kanazawa University,  
Kanazawa (Japan)  
Invited speaker. Page 43

18:00-19:00 Poster Session

19:00-21:00 Free time

21:00 Dinner

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## Tuesday 15 July 2014

### Morning Session Day 2

Session Chair *Rubén Pérez (Universidad Autónoma de Madrid, Spain)*

9:00-9:50 *Molecular-scale Investigations of Solid-Liquid Interfaces by both FM-AFM and 3-Dimensional Force Mapping Method (Part I)*  
**Hirofumi Yamada** Kyoto University, Kyoto (Japan)  
Invited speaker. Page 44

9:50-10:40 *Investigating the contrast mechanisms of AFM and KPFM using functionalized tips (Part I)*  
**Leo Gross** IBM Zurich Research Laboratory, Rüschlikon (Switzerland)  
Invited speaker. Page 45

10:40-11:20 Coffee break

11:20-12:10 *Synthesis at the Single Molecule Level: Chemical Reaction*  
**Michael Crommie** University of California, Berkeley (USA)  
Invited speaker. Page 46

12:10-13:00 *Structure - property by AFM: from atomically defined electromechanical contacts to manipulation of neurons (Part I)*  
**Peter Grutter** McGill University, Montréal (Canada)  
Invited speaker. Page 48

13:00-15:00 Lunch

### Afternoon Session Day 2

Session Chair *José María Gómez-Rodríguez (Universidad Autónoma de Madrid, Spain)*

15:00-15:50 *Advances in quantitative and three-dimensional mapping of soft matter by bimodal force microscopy (Part I)*  
**Ricardo García** Instituto de Ciencia de Materiales de Madrid, CSIC, Madrid (Spain)

	Invited speaker. Page 49
15:50-16:40	<i>Frequency and Bias Spectroscopy and the Use of Multivariate Analysis in Scanning Probe Microscopy (Part I)</i> <b>Stephen Jesse</b> Center for Nanophase Materials Sciences , Oak Ridge National Laboratory (USA) Invited speaker. Page 50
16:40-17:10	Coffee break
17:10-18:00	<i>Forces and photons in molecular tunneling junction.(Part I)</i> <b>José Ignacio Pascual</b> Nanoimaging (CIC9), CIC Nanogune Donostia–San Sebastian (Spain) Invited speaker. Page 51
18:00-19:00	Poster Session
19:00-21:00	Free time
21:00	Dinner

## Wednesday 16 July 2014

### Morning Session Day 3

Session Chair *José María Gómez-Rodríguez (Universidad Autónoma de Madrid, Spain)*

9:00-9:50	<i>Forces and photons in molecular tunneling junction (Part II)</i> <b>José Ignacio Pascual</b> Nanoimaging (CIC9), CIC Nanogune Donostia–San Sebastian (Spain) Invited speaker. Page 51
9:50-10:40	<i>Unraveling nature's secrets with AFM (Part II)</i> <b>Suzanne Jarvis</b> Conway Institute of Biomolecular Research, University College, Dublin (Ireland) Invited speaker. Page 39
10:40-11:20	Coffee break
11:20-12:10	<i>Atom manipulation, single-atom chemical identification and sub-molecular resolution by silicon-cantilever based AFM (Part II)</i> <b>Óscar Custance</b> National Institute for Materials Science, Tsukuba (Japan) Invited speaker. Page 40
12:10-13:00	<i>Instrumentation and applications of liquid-environment FM-AFM (Part II)</i> <b>Takeshi Fukuma</b> Frontier Science Organization Kanazawa University, Kanazawa (Japan) Invited speaker. Page 43
13:00-15:00	Lunch

### Afternoon Session Day 3

Session Chair *Rubén Pérez (Universidad Autónoma de Madrid, Spain)*

15:00-15:50 *Multi-Dimensional Scanning Probe Microscopy with Species-Selective Atomic Resolution Imaging (Part I)*  
**Udo Schwarz** School of Engineering and Applied Science, Yale University, New Haven (USA)  
Invited speaker. Page 52

15:50-16:20 *Physical virology with Atomic Force Microscopy*  
**Pedro J. de Pablo** Universidad Autónoma de Madrid (Spain)  
Invited contribution. Page 53

16:20-16:50 *Advances in Magnetic Force Microscopy*  
**Agustina Asenjo** ICMN-CSIC, Madrid, Spain  
Invited contribution. Page 54

16:50-17:15 Coffee break

17:15-24:00 Visit to the city of Segovia. Dinner in town.

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### Thursday 17 July 2014

#### Morning Session Day 4

Session Chair *Rubén Pérez (Universidad Autónoma de Madrid, Spain)*

9:00-9:50 *AFM experiments with single molecules (Part I)*  
**Ernst Meyer** University of Basel (Switzerland)  
Invited speaker. Page 55

9:50-10:40 *Molecular-scale Investigations of Solid-Liquid Interfaces by both FM-AFM and 3-Dimensional Force Mapping Method (Part II)*  
**Hirofumi Yamada** Kyoto University, Kyoto (Japan)  
Invited speaker. Page 44

10:40-11:20 Coffee break

11:20-12:10 *Synthesis at the Single Molecule Level: Manipulating Structure and Charge*  
**Michael Crommie** University of California, Berkeley (USA)  
Invited speaker. Page 47

12:10-13:00 *Magnetic Sensitive Force Microscopy (Part II)*  
**Alexander Schwarz** Institute of Applied Physics and Interdisciplinary Nanoscience Center, University of Hamburg (Germany)  
Invited speaker. Page 41

13:00-15:00 Lunch

#### Afternoon Session Day 4

Session Chair *José María Gómez-Rodríguez (Universidad Autónoma de Madrid, Spain)*

15:00-15:50 *Simulating Atomic Force Microscopy: (II) Building an AFM simulation.*  
**Adam Foster** Aalto University, Helsinki (Finland)  
Invited speaker. Page 42

15:50-16:40 *Frequency and Bias Spectroscopy and the Use of Multivariate Analysis in Scanning Probe Microscopy (Part II)*  
**Stephen Jesse** Center for Nanophase Materials Sciences , Oak Ridge National Laboratory (USA)  
Invited speaker. Page 50

16:40-17:10 Coffee break

17:10-18:00 *Structure - property by AFM: from atomically defined electromechanical contacts to manipulation of neurons (Part II)*  
**Peter Grutter** McGill University, Montréal (Canada)  
Invited speaker. Page 48

18:00-19:00 Poster Session

19:00-21:00 Free time

21:00 Dinner

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#### Friday 18 July 2014

#### Morning Session Day 5

Session Chair *José María Gómez-Rodríguez (Universidad Autónoma de Madrid, Spain)*

9:00-9:50 *AFM experiments with single molecules (Part II)*  
**Ernst Meyer** University of Basel (Switzerland)  
Invited speaker. Page 55

9:50-10:40 *Investigating the contrast mechanisms of AFM and KPFM using functionalized tips (Part II)*  
**Leo Gross** IBM Zurich Research Laboratory, Rüschlikon (Switzerland)  
Invited speaker. Page 45

10:40-11:00 Coffee break

11:00-11:50 *Advances in quantitative and three-dimensional mapping of soft matter by bimodal force microscopy (Part II)*  
**Ricardo García** Instituto de Ciencia de Materiales de Madrid, CSIC, Madrid (Spain)  
Invited speaker. Page 49

11:50-12:40	<i>Multi-Dimensional Scanning Probe Microscopy with Species-Selective Atomic Resolution Imaging (Part II)</i> <b>Udo Schwarz</b> School of Engineering and Applied Science, Yale University, New Haven (USA) Invited speaker. Page 52
12:40-13:00	Poster awards. Closing remarks. The organizers.
13:00-14:30	Lunch
15:00	Bus to Barajas Airport.

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## **THE SPEAKERS**

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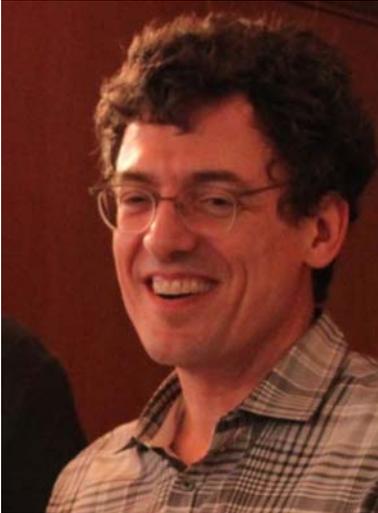
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***INVITED SPEAKER: Michael Crommie***  
***University of California, Berkeley (USA)***



Michael Crommie, Professor at University of California, Berkeley, Department of Physics. Research: Condensed Matter Physics and Materials Science

Mike Crommie received a bachelor's degree in Physics from UCLA in 1984 and his Ph.D. from UC Berkeley in 1991. He was a postdoctoral researcher at IBM Almaden for two years before joining the Physics Department at Boston University in 1994. In 1999 Crommie moved to the Physics Department of UC Berkeley, where he remains today (and where he is also a Lawrence Berkeley National Laboratory Faculty Senior Scientist). Crommie's main research interests lie in exploring the local electronic, magnetic, and mechanical properties of atomic and molecular nanostructures at surfaces. He is interested in studying how interactions between atomic-scale structures affect their microscopic behavior, and how quantum mechanical effects influence device behavior in very small structures

Awards and honors include a National Science Foundation Young Investigator Award (1994), the AAAS Newcomb Cleveland Prize for 1993-94, and a Sloan Foundation Fellowship (1997).

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### ***INVITED SPEAKER: Óscar Custance***

***National Institute for Materials Science, Tsukuba (Japan)***



Oscar Custance got a PhD degree from Universidad Autonoma de Madrid in February 2002 with a doctoral thesis on the study of atomic diffusion and temperature-mediated phase transitions in semiconductor surfaces using variable-temperature scanning tunneling microscopy (STM). Motivated by the potential of atomic force microscopy (AFM) for the study of surfaces with atomic resolution as well as by a marked interest in the Japanese culture, he joined Professor Seizo Morita's Laboratory (Osaka University, Japan) as a postdoctoral researcher in February 2002. During his time at Osaka University, he had the opportunity to participate in landmark works that contributed to push the versatility of the technique, as well as to increase the knowledge on the phenomenology of the interaction between the forefront atoms of the AFM probe and the atoms at semiconductor and insulating surfaces. In February 2008, he got a permanent position at the National Institute for Materials Science (NIMS) (Tsukuba, Japan), where he is currently leading a group devoted to the development of AFM and STM instrumentation as well as the study of materials of technological relevance from an atomistic perspective using these techniques.

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***INVITED SPEAKER: Adam Foster***

***Aalto University, Helsinki (Finland)***



Adam S. Foster (Birmingham, England, 1975) obtained his Masters in Theoretical Physics at Newcastle University, UK in 1997 and his PhD at University College London, UK in 2000. After a post-doctoral position in the Laboratory of Physics, Helsinki University of Technology, Finland he became an Academy of Finland Senior Fellow in 2004 at the same lab. He was appointed Professor at the Department of Physics, Tampere University of Technology, Finland in 2009. In 2012 he returned to Helsinki as a tenured Associate Professor at Aalto University.

Adam S. Foster is the head of the Surfaces and Interfaces at the Nanoscale group (SIN - [physics.aalto.fi/groups/comp/sin](http://physics.aalto.fi/groups/comp/sin)) at Aalto University. The SIN group has extensive experience in simulations of SPM on a wide variety of surfaces, particularly insulating surfaces. The group itself provides comprehensive experience in applying first principles methods for studying nanoscale systems, including both quantum chemical and density functional based approaches, and static and dynamical treatments of atoms and electrons. This is supported by extensive experience in classical atomistic modelling and molecular dynamics. They have performed calculations on a wide variety of systems, including solids, clusters, surfaces and interfaces, and the interaction of these with many different inorganic and organic molecules.

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### ***INVITED SPEAKER: Takeshi Fukuma***

***Frontier Science Organization Kanazawa University, Kanazawa (Japan)***



In 2003, Takeshi Fukuma obtained PhD of engineering at Department of Electronic Science and Engineering, Kyoto University. He spent two years as a postdoc in the department and developed a multi-environment FM-AFM that allows true atomic resolution imaging in vacuum and liquid. From 2005 to 2007, He worked as a Senior Scientist at Physics Department, Trinity College Dublin. During this period, he mainly worked on the improvement of liquid-environment FM-AFM performance and its applications to molecular-scale imaging of biological systems.

In 2007, Takeshi Fukuma started his own group as an associate professor at Frontier Science Organization, Kanazawa University. While he continued to study biological systems by FM-AFM, he developed 3D scanning force microscopy and enabled to visualize 3D distribution of hydration structures at a solid/liquid interface. In 2012, he became a professor at Division of Electrical Engineering and Computer Science, Kanazawa University. Since then, he has been working on the improvement of fundamental performance of FM-AFM.

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### ***INVITED SPEAKER: Ricardo García***

***Instituto de Ciencia de Materiales de Madrid, CSIC, Madrid (Spain)***



Ricardo García Arganza (León), Spain Instituto de Ciencia de Materiales de Madrid, CSIC, Spain (r.garcia@csic.es) <http://www.icmm.csic.es/forcetool/>

Research activity: Garcia applies a combined theoretical and experimental approach to develop multipurpose tools for quantitative analysis and manipulation of molecules, materials and devices in the 1 to 100 nm length scale. A key feature of RG's approach is that nanoscale control and device performance should be compatible with operation in technological relevant environments (air or liquids). He has contributed to the development, understanding and optimization of amplitude modulation AFM (tapping mode). Currently, he participates in the development of bimodal AFM as a unifying scheme for topography and quantitative mapping of material properties with sub-1 nm resolution. He has also contributed to the emergence and optimization of a versatile nanolithography for the fabrication of nano-scale devices, oxidation SPL.

Ricardo García is author or co-author of 122 publications in international peer review journals and 16 book chapters. He has published in a wide range of journals such as Science, Cell, Nature Materials, Nature Nanotech., Nano Lett., Adv. Mater. or Phys. Rev. Lett. RG has an h-index of 41. RG is the author of a book entitled Amplitude modulation AFM, Wiley-VCH (2010). He has co-authored eight patents on nanotechnology instruments and methods. Some of them are commercialized.

#### Awards and Honors

2013, Awarded an ERC Advanced grant

2009, Technological Innovation Prize (1st), Fundación Madri+d, Madrid Regional Government

2007, Fellow American Physical Society (Material Physics), American Physical Society.

1990, Best PhD Thesis in Physics (Universidad Autónoma de Madrid, Spain).

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***INVITED SPEAKER: Franz Giessibl***

***University of Regensburg (Germany)***



Giessibl studied physics from 1982 to 1987 at the Technical University of Munich and at Eidgenössische Technischen Hochschule Zürich. He received a diploma in experimental physics in 1988 with Professor Gerhard Abstreiter and continued with a PhD in physics with Nobel Laureate Gerd Binnig at the IBM Physics Group Munich on atomic force microscopy. After working as a management consultant with McKinsey & Company from 1995 to 1996, he joined Professor Jochen Mannhart at University of Augsburg, where he received a habilitation in 2001.

In 2006, he joined the faculty at the Department of Physics at the University of Regensburg in Germany. Giessibl is a pioneer of atomic force microscopy, who published papers on experimental and theoretical aspects of atomic force microscopy. Giessibl is the inventor of the qPlus sensor, a sensor for Non-contact atomic force microscopy that relies on a quartz cantilever, originally based on quartz tuning forks. Some of his works were the basis for offset prints, such as *Erster Blick* (2000), and *Graphit* (2004) by visual artist Gerhard Richter.

### Awards

1994: R&D 100 Award (together with Brian Trafas)[13]

2000: Deutscher Nanowissenschaftspreis[14]

2001: Rudolf-Kaiser-Preis[15]

2009: Karl Heinz Beckurts-Preis[16]

2010: Ehrenfest Kolloquium Leiden (Netherlands)[17]

2014: Joseph F. Keithley Award for Advances in Measurement Science of the American Physical Society

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***INVITED SPEAKER: Leo Gross***

***IBM Zurich Research Laboratory, Rüschlikon (Switzerland)***



Leo Gross, a native of Berlin, Germany, has been a Research Staff Member at the IBM Research - Zurich Laboratory since 2009. He is working together with Dr. G. Meyer on atomic/molecular manipulation by scanning tunneling microscopy (STM) and atomic force microscopy (AFM), and on nanostencil lithography. He has been with the IBM Research - Zurich Laboratory since 2005. He originally joined IBM Research as a post-doc in the group of Dr. G. Meyer.

Leo Gross received his PhD in Physics in 2005 from the Free University of Berlin in the group of Prof. K.-H. Rieder. And his Master's (Diplom) degree in Physics in 2001 from the University of Muenster, Germany, in the group of Prof. H. Fuchs. Before that, Leo Gross studied one year at the Tulane University, New Orleans, and worked in the group of Prof. U. Diebold. As an undergraduate, he attended the Free University of Berlin.

**Awards:**

Feynman Prize for Nanotechnology, 2012: Awarded by the Foresight Institute. The Feynman Prize for experiment 2012 was awarded to the team of Gerhard Meyer, Leo Gross, and Jascha Repp for their work at IBM Research in Zurich. The award recognizes the experiments advancing the frontiers of scanning probe microscopy.

Gerhard Ertl Young Investigator Award, 2010: Awarded by the Surface Science division of the German Physical Society for the paper entitled "Charge measurement of atoms and atomic resolution of molecules with noncontact AFM".

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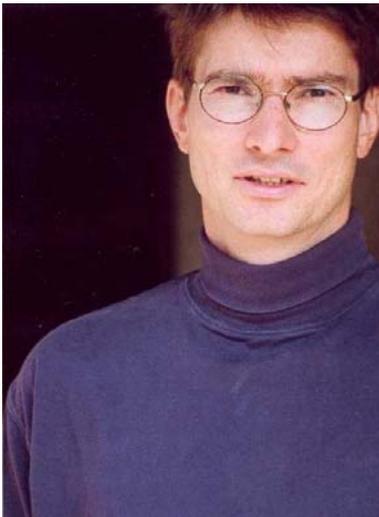
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***INVITED SPEAKER: Peter Grutter***

***McGill University, Montréal (Canada)***



Peter Grutter is chair of the Department of Physics at McGill University in Montreal. He obtained his PhD in 1989 from the University of Basel (Switzerland) and after stays at the IBM Research Centers in Almaden and Zurich joined McGill University in 1994. In 2005, he was elected a Fellow of the Royal Society of Canada, received the Rutherford Memorial Medal in Physics from the Royal Society of Canada, and was awarded the Carrie Derick Award for Excellence in Graduate Teaching and Supervision from McGill University.

His group works on developing scanning probe microscopy based tools and methods and applying them to problems in nanoscience and technology as well as to neuroscience. Research project descriptions and thesis of his group can be found at [www.physics.mcgill.ca/~peter](http://www.physics.mcgill.ca/~peter)

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### ***INVITED SPEAKER: Suzanne Jarvis***

***Conway Institute of Biomolecular and Biomedical Research, University  
College, Dublin (Ireland)***



Suzanne Jarvis graduated from the University of Oxford with a BA in Physics and a Kodak sponsored DPhil in Materials. This was followed by postdoctoral fellowships in Japan at the Joint Research Center for Atom Technology, Tsukuba, before moving on to a staff position at the Nanotechnology Research Institute, also in Tsukuba. During her time in Japan, Suzi co-founded the International Nanotribology Forum, whose mission is to promote the dissemination of nanotribology research with the inclusions of colleagues from developing nations. Suzi moved to Ireland in July 2002 with funding from Science Foundation Ireland to become a Research Professor in the School of Physics at Trinity College Dublin. During her time at Trinity she was one of the founding Principal Investigators at the Centre for Research and Adaptive Nanostructures and Nanodevices. Suzi is currently Professor of Biophysics in the School of Physics, University College Dublin and is based in the Conway Institute for Biomolecular and Biomedical Research. Suzi runs a multidisciplinary team ranging from electrical engineers to botanists. The underlying theme to all her projects is to understand, manipulate and ultimately utilize the function of biomolecules. The group has particular strengths in the development and application of novel atomic force microscopy techniques, especially in the liquid environment.

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### ***INVITED SPEAKER: Stephen Jesse***

***Center for Nanophase Materials Sciences, Oak Ridge National  
Laboratory (USA)***



Stephen Jesse is currently a research staff member at Oak Ridge National Laboratory in the Imaging and Nanoscale Characterization group at the Center for Nanophase Materials Sciences. His current work involves developing novel scanning probe microscopy (SPM) techniques that utilize high-speed electronics and flexible controls to facilitate functional imaging, and increase, by orders of magnitude, the useful information gathered at nanoscale systems. This includes coupling voltage, radio-frequency, and photonic excitation and detections systems to SPM's to extend microscopy to the fundamental time and energy scales of important physical phenomena related to photovoltaic, mechanical, electromechanical, and electrochemical processes. He also works to create new methodologies to analyze and interpret high-dimensional, multi-spectral SPM data.

Stephen received his PhD from the University of Tennessee, Knoxville in Materials Science and Engineering in 2004..

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***INVITED SPEAKER: Ernst Meyer***

***University of Basel (Switzerland)***



Dr. Ernst Meyer is a Professor of physics. He received his Ph.D. at the University of Basel in 1990. The topic of force microscopy on ionic crystals and layered materials was treated in his thesis. He worked at the IBM Research Center Zurich (1992-1994). In 1997, he started his present position at the University of Basel. His research interests are the development of surface science techniques, such as friction force microscopy and dynamic force microscopy with true atomic resolution. He is also active in the field of nanomechanics, including nanotribology and nanosensors. Further probe microscopes, such as Kelvin probe force microscopy, scanning spreading resistance microscopy, scanning force capacitance microscopy and dissipation force microscopy are used to probe dopant concentrations of semiconductors or to investigate novel materials, such as graphene or nanodiamonds.

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### ***INVITED SPEAKER: José Ignacio Pascual***

***Nanoimaging (CIC9), CIC Nanogune Donostia–San Sebastian (Spain)***



Prof. Nacho Pascual obtained his PhD in 1998 at the Autonomous University of Madrid <<http://www.uam.es/ss/Satellite/en/home.htm>> with a Thesis studying the electronic properties of nanometer-sized objects. He was Marie Curie Fellow at the Fritz-Haber Institute <<http://www.fhi-berlin.mpg.de/>> of the Max-Planck-Gesellschaft (2000), Ramon and Cajal Researcher at the Material Sciences Institute of Barcelona <<http://www.icmab.es/>> (2002), and Professor at the Free University of Berlin (2004). From 2010-2013, he was also visiting professor at the “Laboratorio de Microscopias Avanzadas” at the Nanoscience Institute of Aragon <<http://ina.unizar.es/index.php>> (Spain).

Nacho’s main research interest deals with the resolution quantum phenomena at the atomic scale as a method to explore the basic properties of magnetism, mechanics, and electronics. In particular, he has studied the electronic transfer between individual molecules, their interactions and manipulation, and the excitation of their vibrational modes, one molecule at a time. Recently, he has also been interested in effects of the magnetic structure of atoms and molecules interacting with complex materials. From the clear understanding of how atoms and molecules interact and react with their environment, one will be able to design designing the properties of materials.

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***INVITED SPEAKER: Alexander Schwarz***  
***University of Hamburg (Germany)***



Alexander Schwarz (Lübeck, Germany, 22.11.1968), Scientific staff (permanent) in University of Hamburg, Institute of Applied Physics, Hamburg, Germany; obtained his Diploma in Physics (1994) and his PhD (1998) at the University of Hamburg. Since 1998 he has been Senior Scientist responsible for the coordination of the atomic force microscopy activities in the scanning probe microscopy group at the Institute of Applied Physics.

Alexander Schwarz was Member of the steering committee of the "International Conference on Non-Contact Atomic Force Microscopy for fifteen years (Since 1998 to 2012). He has participated in major research activities: Being a principal investigator in the DFG-Collaborative-Research Center (SFB668) "Magnetismus vom Einzelatom zu Nanostruktur" since 2006, and a principal investigator in the ERC Grant "FURORE" (2009-2013). Since 2014 he is a PI in the ERC Grant "ASTONISH". Since 1998 he has supervised four Bachelor students, one Master student, thirteen Diploma students and fifteen PhD students.

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***INVITED SPEAKER: Udo Schwarz***

***Yale University, New Haven (USA)***



Udo D. Schwarz, Professor of Mechanical Engineering and Materials Science and Chemical and Environmental Engineering, Yale University

Udo D. Schwarz graduated in 1989 from the University of Basel, Switzerland, receiving his Ph.D. in physics from the same institution in 1993. Subsequently, he continued his work as a staff scientist and lecturer at the Institute of Applied Physics of the University of Hamburg, Germany. In 2001, Prof. Schwarz moved to the Materials Science Department of the Lawrence Berkeley National Laboratory in Berkeley, California. Since 2002, he works at Yale's Mechanical Engineering Department, where he got promoted to full professor in 2009 and department chair in 2012.

His research interests concern the local measurement of various atomic-scale interactions and properties, including electric, magnetic, chemical, and nanotribological interactions. More specifically, he uses scanning probe microscopy techniques (predominantly scanning force microscopy) to study problems in surface physics, catalysis, friction, adhesion, and the physics of dielectrics, semiconductors, and metals.

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### ***INVITED SPEAKER: Hirofumi Yamada***

***Kyoto University, Kyoto (Japan)***



Prof. Hirofumi Yamada received a B.S. degree in 1980 and a Master of Science in 1982, from Kyoto University. He received his PhD in engineering (Department of Applied Physics), from University of Tokyo with the Thesis: "Atomic Force Microscopy of Organic Materials" in 1994

Hirofumi Yamada worked for the Space Communication Division, Hitachi Ltd. From 1982 to 1984. From this date to 1993 he developed his career as Research Associate in the National Research Laboratory of Metrology, Agency of Industrial Science and Technology/MITI. From 1989 to 1991 he was at E. L. Ginzton Laboratory, Stanford University as a visiting researcher. After that, he worked as Senior researcher at Joint Research Center for Atom Technology, in the National Institute for Advanced Interdisciplinary Research, Agency of Industrial Science and Technology/MITI. From 1996 he has been Associate Professor in the Kyoto University

Hirofumi Yamada has been Visiting professor at Osaka University (2003) and University of Tokyo (2004). He has been Chairman of Advanced Nanoprobe Technology Research Committee, (Foundation Advanced Technology Institute: ATI), from 2003, and he has organized several International conferences (Non-contact Atomic Force Microscopy 2001 (NC-AFM2001, Kyoto); Scanning Tunneling Microscopy 2005 (STM2005, Sapporo); Non-contact Atomic Force Microscopy 2005 (NC-AFM2005, Osnabrück); Int'l Symposium on Surface Science & Nanotechnology (ISSS-4, Omiya)

#### Honors and Awards:

2004 Nanoprobe Technology Award of Nanoprobe Committee of Jpn. Soc. for Promotion of Sci. (JSPS)

2008 Technology Award of The Surface Science Society of Japan.

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***INVITED CONTRIBUTION: Agustina Asenjo***  
***ICMM-CSIC, Madrid (Spain)***



Agustina Asenjo is a researcher of the Instituto de Ciencia de Materiales de Madrid-CSIC with extended experience in SPM, particularly Magnetic Force Microscopy and in the fabrication and characterization of nanomagnets. She has contributed to the introduction in Spain of Magnetic Force Microscopy.

Agustina Asenjo is co-author of 77 publications in international peer review journals, with more than 800 citations (h-index of 17). She is also co-author of one book chapter. AA is nowadays deputy director of the ICMM-CSIC.

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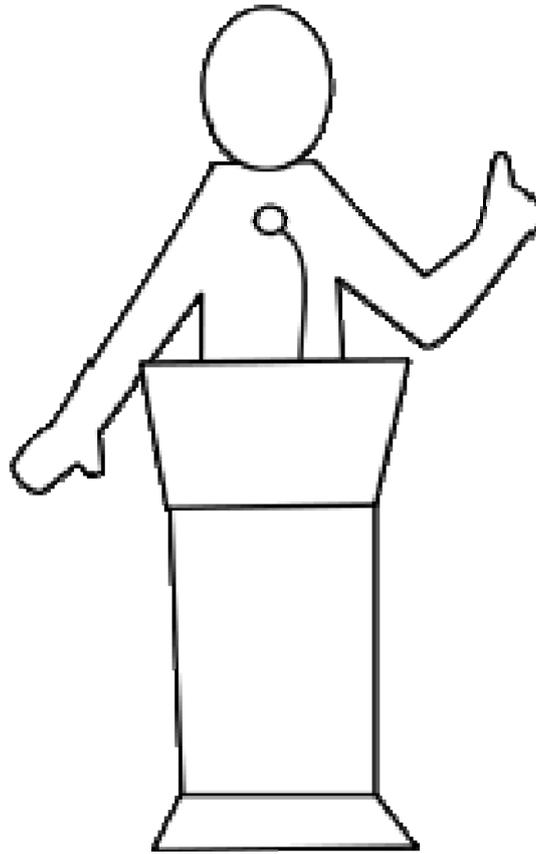
### ***INVITED CONTRIBUTION: Pedro J. de Pablo***

***Universidad Autónoma de Madrid (Spain)***



Pedro José de Pablo Gómez, was born in Madrid (Spain) and studied Physics at Universidad Autónoma de Madrid. He performed the PhD at the same university, and obtained the Extraordinary PhD prize in 2000, as one of the best thesis of the University. He enjoyed several internships at the department of Physics of Purdue University (USA). In September 2001 he moved to The Netherlands to carry on postdoctoral research on single-molecule biophysics at the Vrije Universiteit under the supervision of Prof. Christoph Schmidt. In 2003 Pedro started his own independent group at Universidad Autónoma de Madrid supported by the Spanish Ramón y Cajal program. In 2011 he gained a position of Associate Professor at the Universidad Autónoma de Madrid. Pedro is currently teaching General Physics for Biology, Thermodynamics for physicists and he is also involved in the UAM Biophysics Master as experimental techniques teacher.

Pedro's research has multidisciplinary character, since he has been involved in investigating a wide range of phenomena, including from electromigration and electronic transport in mesoscopic structures, such as carbon nanotubes and DNA, to the study of molecular motors and viruses with Atomic Force Microscopy. He has developed new AFM methods such as jumping mode and non-contact electrostatic methods based on non-intrusive dynamic AFM modes. During the postdoctoral stage with Prof. Christoph Schmidt at Vrije Universiteit Pedro introduced Atomic Force Microscopy, adapting this technique in two different projects. The first one regarded on following the activity of single molecular motors, such as kinesin on microtubules, with AFM working in liquid milieu. The second project dealt with the mechanical properties of two molecular aggregates such as microtubules and phage  $\phi 29$  in vitro conditions. The publication in PNAS about the  $\phi 29$  bacteriophage, where Pedro is coauthor, is a seminal work that initiated a new research line all-over the world consisting on investigating the mechanical properties of viruses and their implication in the viral biophysics.



## **ABSTRACTS. ORAL PRESENTATIONS**

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## Atomic Force Microscopy at the Picoscale

Franz J. Giessibl

Experimental and Applied Physics, University of Regensburg, 93053 Regensburg,  
Germany

Email: [fgiessibl@yahoo.com](mailto:fgiessibl@yahoo.com)

Heinrich Rohrer stated in his Nobel lecture [1], that measuring discontinuities of Young's modulus at the superconducting transition made him lose all respect for Angstroms. He and Gerd Binnig left big footsteps, and in following their tracks, picometers, picoamperes and piconewtons became the new yardsticks in science at the atomic and subatomic scale. The challenges in this arena are noise reduction in physical measurements as well as the quantum nature of matter.

Atomic force microscopy faces a special challenge. Tip-sample distances are typically much smaller than in scanning tunneling microscopy for two reasons: first, small forces are harder to measure than small currents and second, tip-sample forces contain long range components, and the relative contribution of short range versus long range force becomes greater when choosing smaller tip-sample distances. As a consequence, effects of the force on the probing atom or CO terminated tip become noticeable. Combining atomic force microscopy with tunneling microscopy (or vice versa), such as easily possibly by using the qPlus sensor has the appeal to address conducting and nonconducting states of solids at the same time (see figure).

References:

[1] [http://www.nobelprize.org/nobel\\_prizes/physics/laureates/1986/rohrer-bio.html](http://www.nobelprize.org/nobel_prizes/physics/laureates/1986/rohrer-bio.html)

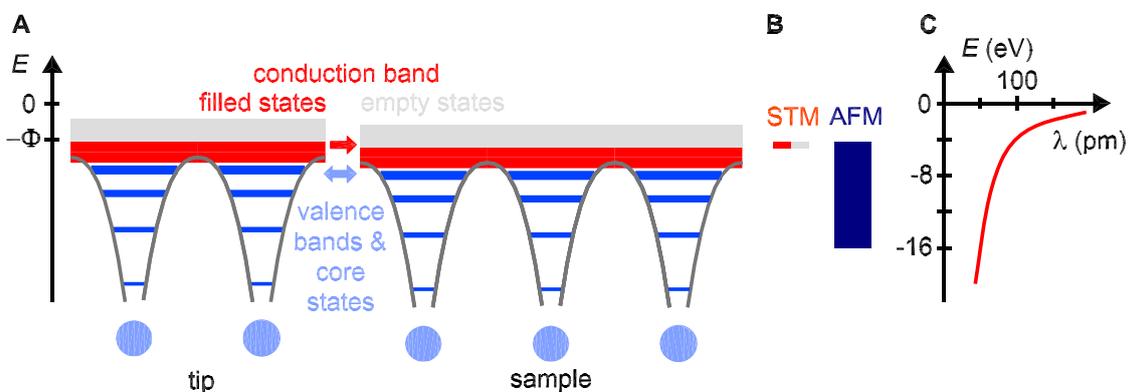


Fig 1. Fig. S11 from Welker & Giessibl, *Science* **336**, 444 (2012)

## **Unraveling nature's secrets with AFM**

Suzi P. Jarvis

UCD Conway Institute, University College Dublin, Dublin 4, Ireland.

E-mail: [suzi.jarvis@ucd.ie](mailto:suzi.jarvis@ucd.ie)

(1) Using an atomic force microscope (AFM) it is possible to delicately pull apart protein structures in order to characterize their mechanical properties and thus provide a molecular level explanation for their mechanical strength. Pulling apart protein structures in a systematic way enables us to build up a series of characteristic force-extension curves for molecules and fibres. By analyzing such curves using worm like chain analysis we can extract quantitative information and identify underlying structural differences.

In this presentation we explore the experimental techniques and analysis of protein pulling experiments and discuss how this information may be used to characterize biomaterials of interest.

## **Atom manipulation, single-atom chemical identification and sub-molecular resolution by silicon-cantilever based AFM**

Oscar Custance

National Institute for Materials Science (NIMS), Sengen 1-2-1, 305-0047 Tsukuba,  
Japan

[CUSTANCE.Oscar@nims.go.jp](mailto:CUSTANCE.Oscar@nims.go.jp)

Since the first demonstration of atomic resolution imaging using dynamic AFM [1], several landmark works have contributed to push the resolution limits [2-4] and versatility [5-10] of this technique. Some of these accomplishments were carried out using commercial micro-fabricated silicon cantilevers driven at nanometer-range oscillation amplitudes as force sensors, in contrast to the current general trend in the field of using stiff piezoelectric cantilevers and sub-angstrom oscillation amplitudes. Here, we will introduce some of our accomplishments using silicon-cantilever based AFM. We will describe some of the pioneering works that demonstrated the atomic manipulation capabilities of AFM [6, 11]. We will also explain a method for the chemical identification of individual atoms, which is based on the precise quantification of the interatomic forces [5] between the foremost atom of the AFM probe and the surface atoms [7]. Finally, we will propose a method for high-resolution imaging of three-dimensional surface structures using a silicon-cantilever based AFM [12]. We demonstrate this method by visualizing the structure of a pentacene molecule together with the atomic positions of the substrate, and by resolving the contour and probe-surface force field on a C60 molecule with intra-molecular resolution [4]. We will show that this method is particularly useful to characterize atomic steps of reactive surfaces (where AFM imaging is challenging) and study the adsorption of molecular species at surface steps.

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- [3] U. Kaiser, A. Schwarz, R Wiesendanger, *Nature* **446**, 522 (2007)
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- [6] Y. Sugimoto et al., *Nature Mater.* **4**, 156 (2005)
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- [10] B. Albers et al., *Nature Nanotech.* **4**, 307 (2009)
- [11] Y. Sugimoto et al., *Science* **322**, 413 (2008)
- [12] C. Moreno et al., (*submitted*)

# Magnetic Sensitive Force Microscopy

Alexander Schwarz

Institute of Applied Physics, University of Hamburg, Jungiusstr. 11, D-20355 Hamburg  
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Magnetism is one of the most important physical phenomena utilized by humans. It was known to the ancient Greeks as well as ancient Chinese. The latter used them for naval navigation already about 1000 years ago. Today, most of the total amount of recorded data on planet earth is stored magnetically. Moreover, many sensing devices, apart from hard disks read-write heads, are actually based on magnetic effects. Naturally, scanning probe techniques has been applied to study magnetism very early on.

In this lecture I will first explain some basics on magnetism, e.g., its atomistic origin, magnetism in solids, the Heisenberg model, spin-orbit coupling and magnetic anisotropy energies, hysteresis and magnetization reversal etc. Thereafter, magnetic force microscopy (MFM) will be introduced. It has been developed in 1987 [1], only one year after the invention of atomic force microscopy, and since then applied to study domain structures in ferromagnetic thin films (recording media), small magnetic particles (single domain vs. multi domain state) and artificially patterned structures (spin ice, magnetic monopoles). Moreover, flux lines in superconductors have been investigated (vortex matter). However, as MFM probes the stray field above the surface, its spatial resolution is limited to about 10 nm.

Atomic resolution requires another technique, namely magnetic exchange force microscopy (MExFM), where the tip sample distance is below 1 nm, so the magnetic exchange interaction via an overlap of the spin carrying orbitals in tip and sample can be detected. Although this possibility was mentioned as early as 1990 [2], its feasibility was proven only 2007 [3]. Up to now, only antiferromagnetically ordered surfaces have been studied [3,4,5], but non-collinear spin structures should be observable as well. Additionally, its spectroscopic mode, i.e., magnetic exchange force spectroscopy (MExFS), allows determining magnitude and distance dependence of the magnetic exchange interaction quantitatively [6]. This information can then further employed to induce magnetic switching via adjusting an appropriate tip-sample separation [7].

## References

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# Simulating Scanning Probe Microscopy

Adam S. Foster

COMP, Department of Applied Physics, Aalto University, Helsinki, Finland  
E-mail: adam.foster@aalto.fi

As surface science has increasingly moved to the nanoscale over the past decade, it has entered a realm that is also accessible to highly accurate computational approaches. Simulations have become a key partner in many studies, with the interplay between theory and experiment being the critical element in real understanding. This is especially true in Scanning Probe Microscopy (SPM), where joint experimental and theoretical studies are common [1,2].

In this lecture, I will try to introduce the most popular tools used in computational surface science, along with examples highlighting their interaction with experiment. I will also show examples where common methods fail, and point out the consequences of some “short-cuts” often hidden in the technical details. From this, I will walk through the stages of building a simulation of SPM, with the details mostly relevant to modelling of noncontact Atomic Force Microscopy (AFM) in UHV. We will also touch on some the issues involved in modelling of more complex systems, such as dissipation [3], kelvin probe microscopy [4] and AFM in liquids [5].

## References:

- [1] W. Hofer, A. S. Foster and A. L. Shluger, *Rev. Mod. Phys.* **75**, 1287 (2003).
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## Instrumentation and applications of liquid-environment FM-AFM

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Frequency modulation atomic force microscopy (FM-AFM) has traditionally been used in vacuum for atomic-scale studies on various materials including insulators as well as conductive and semiconducting materials. However, recent progress in the instrumentation<sup>1</sup> has enabled its operation in liquid with true atomic resolution<sup>2</sup>. This technical innovation has enabled subnanometer-scale imaging of biological molecules<sup>3</sup>. Furthermore, combined with subsequently developed three-dimensional (3D) force measurement techniques, FM-AFM has enabled 3D measurements of hydration structures<sup>4</sup> and flexible surface structures at solid/liquid interfaces<sup>5</sup>. In the meanwhile, instrumentation work has made further improvements in the fundamental performance of FM-AFM. The use of small cantilevers with a resonance frequency of 3.5 MHz in liquid has been realized by developing a stable photothermal excitation system with temperature control<sup>6</sup>. The use of the small cantilever has significantly improved the force resolution and time response of FM-AFM. A digital phase-locked loop (PLL) circuit with an improved algorithm has significantly improved the measurement bandwidth of FM-AFM<sup>7</sup>. Combined with the small cantilever, the developed PLL has enabled high-speed and atomic-resolution imaging of calcite crystal growth process at 1 frame/sec in water<sup>8</sup>. In this presentation, I would like to review these recent progresses in the instrumentation and applications of liquid-environment FM-AFM.

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# Molecular-scale Investigations of Solid-Liquid Interfaces by both FM-AFM and 3-Dimensional Force Mapping Method

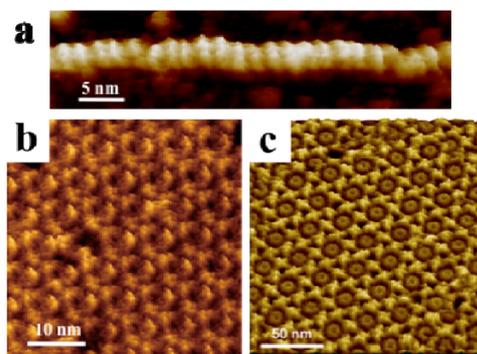
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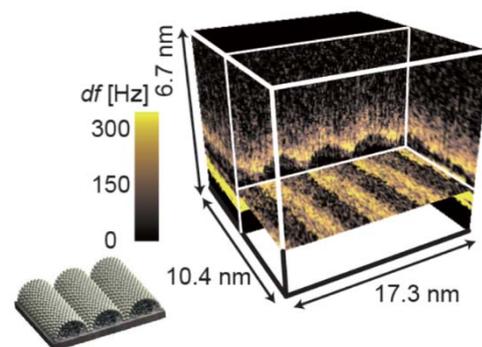
Solid-liquid interfaces play a critical role in a large variety of physical, chemical and biological processes, such as crystal growth, catalytic reactions and various biochemical functions. Investigations of molecular-scale structures and interactions at solid-liquid interfaces are, therefore, essentially crucial for understanding these microscopic processes. Recent, significant progress in FM-AFM working in liquids has allowed us to directly study such molecular-scale processes, including various “in vivo” biological interactions. In this presentation, we first discuss the fundamental noise character in FM-AFM in low Q-factor environment which is an essential factor to determine the minimum detectable force and the special resolution[1]. Some recent results on high-resolution FM-AFM imaging of biomolecules in physiological environments [2,3] are also presented. In addition, we describe the visualization of 2D/3D molecular-scale hydration structures at solid-liquid interfaces as well as those around biomolecules, which were obtained by force mapping method based on FM-AFM. The technique has been also applied to the visualization of local electric double layer (EDL) forces on molecular assemblies in electrolyte solution. Since we used the photothermal excitation for the cantilever oscillation, the EDL forces can be quantitatively measured. In fact we successfully obtained the molecular-scale surface charge density utilizing a modified DLVO (Derjaguin, Landau, Verwey and Overbeek) theory [4].

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**Fig. 1.** FM-AFM images of DNA double-helix structure, hexagonal array of *bacteriorhodopsin* trimers(b), and 2D crystal of IgG antibody hexamers(c).



**Fig. 2.** 3D-visualization of EDL force on SDS surfactant molecular assemblies. (Bottom left) Model of SDS surface micelles.

## Investigating the origin of atomic contrast with AFM and KPFM using functionalized tips

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Tip functionalization is crucial for achieving atomic resolution with atomic force microscopy (AFM) on molecules [1,2]. Depending on the properties to be measured different tip functionalizations are preferable (see Fig. 1). Tips terminated with CO yield high apparent resolution and are suited even for bond-order discrimination [3]. However, the molecular images appear distorted due to the tilting of the CO molecule at the tip apex. On the other hand Xe tips yield images that show less contrast but these can be used for a precise determination of the adsorption geometry of individual molecules [4].

Recent results on atomic resolution with Kelvin probe force microscopy (KPFM) on molecules [5,6] and ionic systems are discussed. Different tip functionalizations in combination with force-distance spectroscopy and force-voltage spectroscopy are employed to investigate the basic contrast mechanisms for AFM and KPFM on the atomic scale.

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Fig. 1

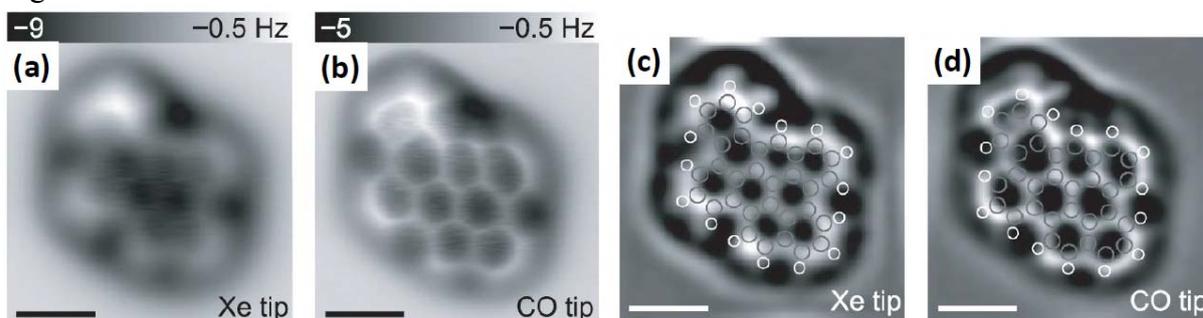


Fig. 1: Constant-height NC-AFM measurements of dibenzo-naphtho-perylene on bilayer NaCl on Cu(111) using (a) a Xe tip and (b) a CO tip. (c,d) Laplace and low-pass filtered versions of (a,b), respectively, with calculated atomic positions overlaid. Scale bars: 5 Å. Reproduced from Ref. [2].

## Synthesis at the Single Molecule Level: Chemical Reaction

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Progress in molecular self-assembly at surfaces has enabled fabrication of increasingly complex molecular nanostructures. This includes graphene-based nanoribbons fabricated via step-growth polymerization from chemically-engineered monomer precursors. The chemical route that is typically used here (and for many other surface molecular structures) involves halide cleaving of the precursors to form radicals which then undergo polymerization, and then dehydrogenation/cyclization in the case of nanoribbons (to form full aromatic  $\pi$ -bonded networks). This technique is limited by the fact that it typically requires a metal surface in order to catalyze the halide cleaving step. In order to eventually overcome this limitation we are exploring other surface chemical routes to polymerization and cyclization that do not involve a halide cleaving step. One possible route involves Bergman cyclization of monomers to directly form radicals which can then undergo polymerization and additional cyclization. We have explored the use of enediyne molecular fragments on surfaces to perform these reactions. We have used STM and AFM techniques to explore cyclization and polymerization processes for this class of molecules, and we have identified different cyclization and polymerization pathways. New qPlus imaging techniques have allowed us to directly image chemically intermediate structures and to gain new insights into the role that surface dissipation plays in mediating molecular self-assembly.

## Synthesis at the Single Molecule Level: Manipulating Structure and Charge

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Controlling the precise placement of charge in molecular-scale structures is an important goal in order to create new types of electronic and magnetic devices down to the ultimate atomic limit. Because molecular structures are smaller than typical semiconductor quantum dots, their charging energies are larger and they have the potential for higher-temperature operation. Molecular structures have previously been placed into gated devices in order to explore their charging behavior via transport, but the precise microscopic structure of those systems was unknown due to an inability to image the molecules in a device environment. Conversely, microscopic charging behavior of molecules on metal surfaces has been imaged previously using STM, but this has typically been in geometries that cannot be electrostatically gated. New experiments will be discussed here that involve the exploration of individual and self-assembled molecules adsorbed onto the surface of a back-gated graphene device. Such a substrate is unique for single-molecule surface investigations in that it can be electrostatically gated, thus changing the charge-state of the supported molecules. Molecular adsorbates were chosen for this work that have an orbital that energetically aligns close to the graphene Dirac point so that the molecular charge-state can be manipulated via the electrostatic back-gate. Using this arrangement we have observed Anderson impurity behavior for individual molecules as they "snap" from neutral non-magnetic states to charged magnetic states under the influence of the graphene back-gate. When the molecules are arranged into assemblies on the gated graphene surface observe patterned charge formations that arise due to molecule-molecule Coulomb interactions. STM techniques allow us to observe the molecular electronic behavior while AFM techniques allow us to observe the precise molecular structure. Combined STM/AFM measurements provide new insight into molecular structure/function relationships.

# Structure – property by AFM: from atomically defined electromechanical contacts to manipulation of neurons

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Atomic Force Microscopy (AFM) is a technique that allows atomic scale spatial resolution on essentially any material, including insulators and metals, in essentially any environment: from ultra high vacuum to liquids, at temperatures of several 100K down to mK. These images allow extraction of detailed structural information, in particular when combined with state of the art modeling. Many properties, such as electrical surface potential, elasticity, yield stress, adhesion or friction can be measured and correlated to structure, often as a function of external parameters such as light or electrochemical potential. Completing this ‘nanolab’ is the capability of AFM to manipulate objects. In this summer school I will concentrate on structure-property AFM experiments that can give us fundamental insights in fields which have major potential for important applications. Some of the fundamental questions we are trying to address are: how is charge separated in organic photovoltaics? What determines Li mobility in batteries? How does the electrical conductivity of a nanometer scale contact depend on mechanical properties? What induces the formation of a synapse in a neuron? By describing my research group’s ongoing attempts to find answers to these questions I will also demonstrate how state-of-the-art AFM goes well beyond being a tool to make ‘pretty’ images.

References:

For a complete list of our publications please see [www.physics.mcgill.ca/~peter](http://www.physics.mcgill.ca/~peter)

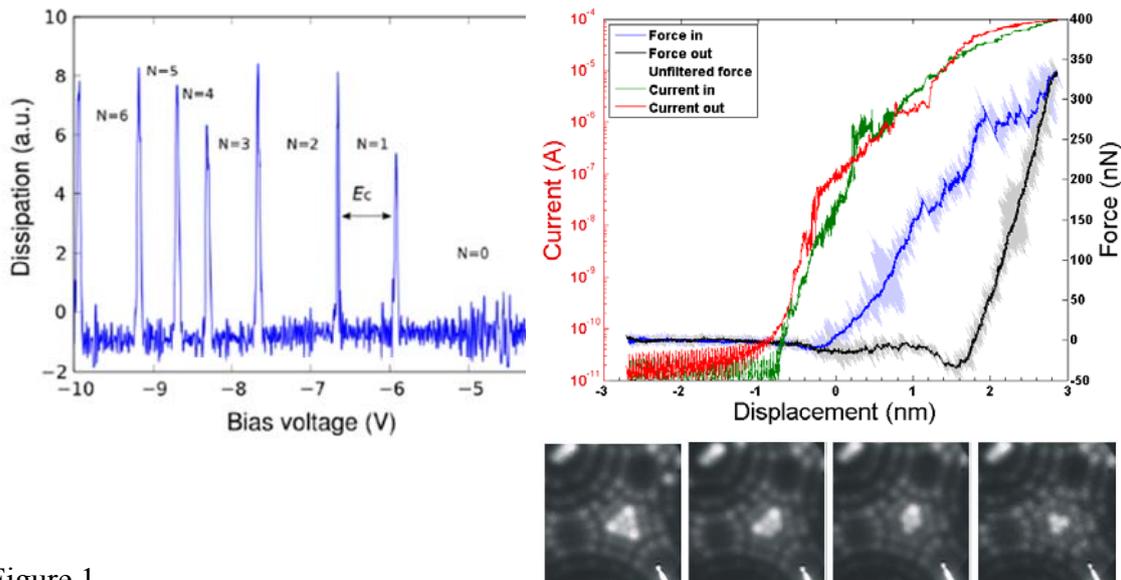


Figure 1.

*Above:* Single electron spectroscopy by AFM

*Right:* Investigation of electronic and mechanical properties using an atomically defined contact.

# Advances in quantitative and three-dimensional mapping of soft matter by bimodal force microscopy

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Force microscopy is considered the second most relevant advance in Materials Science since 1960. Despite the success of AFM, the technique currently faces limitations in terms of three-dimensional imaging, spatial resolution, quantitative measurements and data acquisition times. Atomic and molecular resolution imaging in air, liquid or ultrahigh vacuum is arguably the most striking feature of the instrument. However, high resolution imaging is a property that depends on both the sensitivity and resolution of the microscope and on the mechanical properties of the material under study. Molecular resolution images of soft matter are hard to achieve. In fact, no comparable high resolution images have been reported for very soft materials such as those with an effective elastic modulus below 10 MPa (isolated proteins, cells, some polymers). Similarly, it is hard to combine the exquisite force sensitivity of force spectroscopy with molecular resolution imaging. Simultaneous high spatial resolution and material properties mapping is still challenging.

This presentation reviews some of the above limitations and some recent developments based on the bimodal operation of the AFM to address and overcome them

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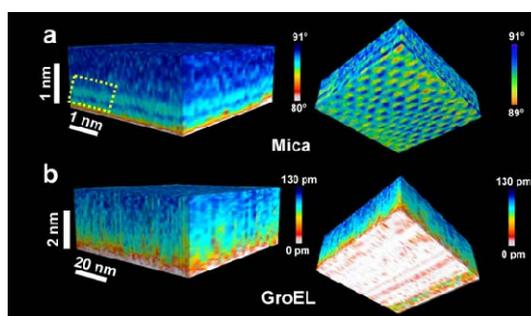


Fig. 1. Bimodal AFM 3D images of solid-water volumes. a, 3D map of a mica-water interface. The stripes are associated to the presence of hydration layers. b, 3D map of a GroEL patch-water interface. The side view shows a slightly rough landscape with variations of the amplitude of about 1 nm.

# **Frequency and Bias Spectroscopy and the Use of Multivariate Analysis in Scanning Probe Microscopy**

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Scanning probe microscopy offers a unique tool for probing nanoscale dynamic phenomena in solids ranging from phase transitions to electrochemical reactions – targets of crucial importance for material science. In these experiments, the SPM tip focuses an electric or thermal field or other excitation field to a nanoscale region of material, inducing local transformations. Simultaneously, tip-surface current and multi-frequency excitation and detections methods are used to measure dynamic strain, resonance frequency shifts, quality factor, and transport properties to provide information on processes in the material (polarization, domain formation, ionic and electronic motion, surface charging, and second phase formation, melting) induced by local stimulus. Highly localized spectroscopy offers particular advantages for materials research in that transformations can be probed in material volumes containing no or single individual defects, paving a pathway for studying phase transformations and electrochemical reactions on the single defect level. Discovering and differentiating the various phenomena occurring at the tip-surface junction requires the implementation of complex spectroscopic methods. Therefore, these studies require improvement in capability to collect and analyze multidimensional data sets necessary to capture time- and field-dependent behavior at each spatial location. I will discuss several SPM based approaches for probing dynamic bias-induced phenomena at solid-gas and solid-liquid interfaces, including reversible and irreversible electrochemical reactions, intercalation, and ionic migration. I will further illustrate the use of data mining methods based on multivariate statistics, such as principal component and Bayesian analysis, supervised and non-supervised learning for analysis of the multidimensional data and some strategies for matching with theoretical models.

This research was conducted at the Center for Nanophase Materials Sciences, which is sponsored at Oak Ridge National Laboratory by the Scientific User Facilities Division, Office of Basic Energy Sciences, U.S. Department of Energy.

# Force spectroscopy at the molecular scale

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Force spectroscopy has extended our toolset for resolving electrostatic and mechanical properties of individual molecules with sub-molecular resolution. This particularly remarkable when combined with tunneling electron spectroscopy, because it allows us to identify the conformational states associated to certain transport modes. In this presentation, I will review several works of our laboratory making use of a qPlus-based non-contact AFM/STM regarding electronics, electrostatics and mechanics of molecular tunnel junctions.

- The formation of a molecular junction involves the formation of bonds and interactions. Using point force spectroscopy we trace the formation of a non-covalent bond between two molecules, revealing the very important role of electrostatics.

- Capacitive force measurements are used to uncover the dipolar distribution of molecules with intrinsic dipole moment.

- Molecular conformational changes are followed during the formation of molecular bridges between the tip of the STM and the surface. Here, we measure forces revealing the intramolecular flexibility and deformations occurring during the formation of the molecular junction. We resolve the strong effect that specific conformations cause in the transmission through the junction.

- The stochastic motion of a bi-stable molecule can be induced by inelastic tunneling electrons. We identify these conformational changes through the forces exerted on the tip. The effect of bi-stabilities in the structure of a molecular junction will be addressed [1].

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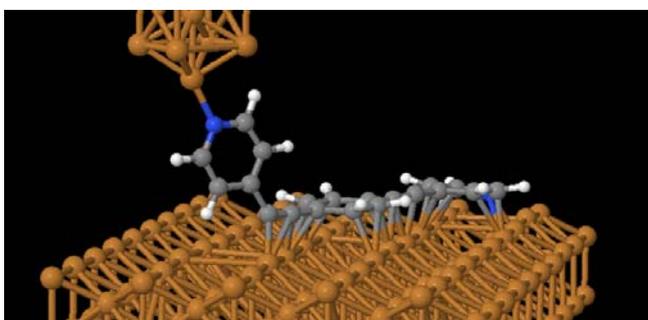


Figure 1

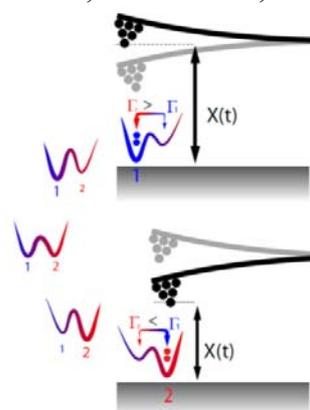


Figure 2

\* In representation of his colleagues from the Freie Universität Berlin and nanoGune: Christian Lotze, Martina Corso, Nils Krane, Fabian Schulz, Gunnar Schulze, JingChen Li, Katharina Franke

# Multi-Dimensional Scanning Probe Microscopy with Species-Selective Atomic Resolution Imaging

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Despite the evolution of scanning probe microscopy (SPM) into a powerful set of techniques that image surfaces and map their properties down to the atomic level, significant limitations in both imaging and mapping persist. Currently, typical SPM capabilities qualitatively record only one property at a time and at a fixed distance from the surface. Furthermore, the probing tip's apex is chemically and electronically undefined, complicating data interpretation. To overcome these limitations, we started to integrate significant extensions to existing SPM approaches. First, we extended noncontact atomic force microscopy with atomic resolution to three dimensions by adding the capability to quantify the tip-sample force fields near a surface with picometer and piconewton resolution [1-4]. Next, we gained electronic information by recording the tunneling current simultaneously with the force interaction [5]. We then moved on to study the influence of tip chemistry and asymmetry on the recorded interactions [4, 6]. Through a combination of experimental work and theoretical analysis, we show how specific atomic species can be selectively imaged in both the force and the current channels depending on the choice of imaging parameters and tip chemistry. Applications to metal oxides are shown. From this platform, we present our vision of a method capable of characterizing full atomic-scale chemical and electronic properties.

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# Physical virology with Atomic Force Microscopy

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Viruses are striking examples of macromolecular assembly of proteins, nucleic acids, and sometimes lipid envelopes that form symmetric objects with sizes ranging from 10 to 100s of nanometers. The basic common architecture of a virus consists of the capsid a protein shell made up of repeating protein subunits, which packs within it the viral genome which can be single or double stranded DNA or RNA depending on the type of the virus. Virtually every aspect of the virus cycle from DNA packing to maturation to interaction with the host modifies and, in turn, is influenced by the material properties of the virus. In this talk I will show how Atomic Force Microscopy has emerged as a unique technique to unveil some physical properties of viruses (1,2), such as stiffness and elasticity, which can be directly related to their structure and function (3,4). In addition, AFM enables monitoring the dynamics of virus disassembly in real time to unveil the ultimate physical changes to trigger virus infectivity (5).

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## Advances in Magnetic Force Microscopy

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More than 25 years after its invention, the Magnetic Force Microscopy (MFM) has become a widespread tool to characterize magnetic materials and structures at nanoscale. However, the impact of the technique is limited due to the possible influence of the tip stray field on the sample configuration and the challenging task of providing quantitative data about the sample magnetization.

In the present work, MFM-based techniques developed in our group are described. The Variable-Field MFM allows imaging under variable magnetic fields in order to gain information about reversal magnetization processes [1,2]. An application of this VFMM are used to obtain the hysteresis loops of MFM probes and individual nanostructures [3]. In the last years, Kelvin Probe Force Microscopy (KPFM) has been combined with MFM in order to distinguish the electrostatic and magnetic tip-sample forces and moreover to separate both contributions which is crucial in low magnetic moment materials [4,5]. Finally, we will present recent results about the study of magnetic dissipation processes in MFM [6] and how to extract information about the magnetic properties of the sample.

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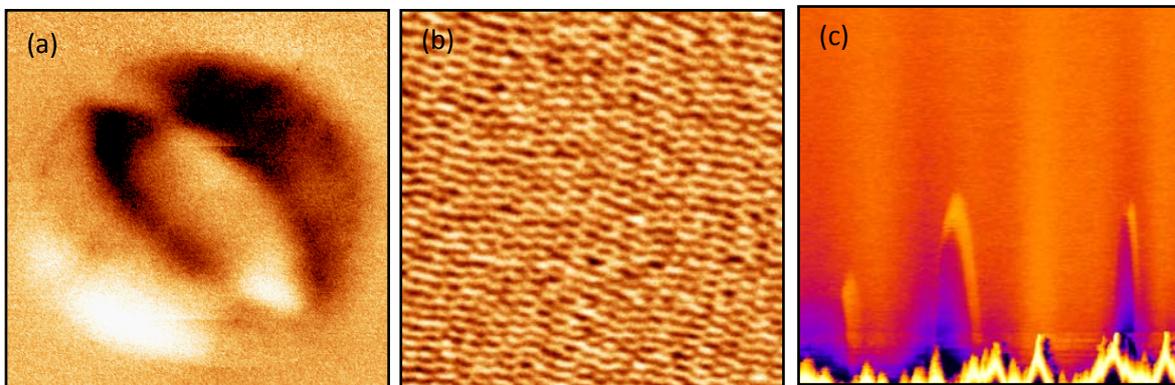


Fig. 1: (a) VFMM image of a Co dot. (b) High resolution MFM image of a HDD. (c) Dissipation versus distance image obtained in CoNi sample.

# Force microscopy experiments with single molecules

Ernst Meyer<sup>1</sup>

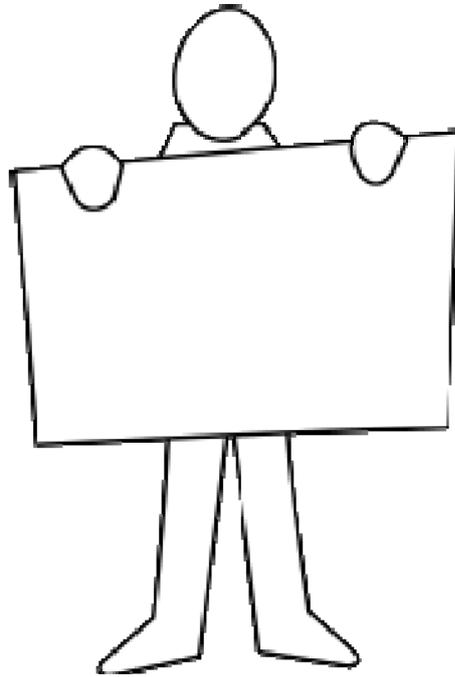
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Non-contact force microscopy has demonstrated true atomic resolution on metals, semiconductors and insulators. The application of AFM to single molecules is a challenge because of relatively weak bonding to the substrate, which often leads to high diffusion rates of the molecules. We will present molecules, which were designed to interact with specific sites on insulating surfaces. Molecular wires of porphyrin molecules on ionic crystal surfaces are observed. A complete immobilization at kink sites of KBr(001) is observed for single truxene molecules at room temperature [1]. Recently, intramolecular resolution is studied on a variety of molecules [2]. A further challenge is the manipulation of molecules on surfaces, including the controlled rotation, which means that the direction of rotation of the molecule can be chosen by the experimentalist [3]. The control of the probing tip is of central importance for a quantitative understanding of nc-AFM imaging and force spectroscopy. Progress has been made by a variety of preparation procedures: sputtering, indentation or pick-up of molecules, such as CO. The attachment of a single molecule to the end of the tip is shown for the case of a functionalized porphyrin, which can be used as a stable probing tip for imaging in the attractive as well as the repulsive regime. The on-surface synthesis of long polymeric wires gives the opportunity to study the detachment of more complex molecules, where the simultaneous measurement of force and tunneling currents gives a rich variety of information about the molecular wire and its interaction with the surface [5].

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## **ABSTRACTS. POSTER PRESENTATIONS**

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# XX International Summer School "Nicolás Cabrera"

## Biomolecules and Single-Molecule Techniques

Madrid, Spain, 21-26 July 2013

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## P1

**CONSTANT AMPLITUDE -DSFM AS ONLY REASONABLE  
DYNAMIC SFM MODE WITH -ATTRACTIVE AND REPULSIVE-  
SURFACES IN LIQUIDS**Lisa Almonte<sup>1</sup>, Arturo M. Baró<sup>1</sup>, Jaime Colchero<sup>2</sup><sup>1</sup>Intituto de Ciencia de Materiales de Madrid-CSIC, Campus de Cantoblanco E-28049  
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Scanning Force Microscopy (SFM) is a powerful tool in the field of Biology and Biophysics due to its ability to image and measure forces (Van der Waals, electrostatic or deformation forces) of in-vivo biological samples in physiological environment. The biological samples in liquid medium have a surface charge that may be repulsive or attractive regarding SFM tip according to the ionization of molecules in the medium with a specified pH. To modify or damage the sample as little as possible is important to measure in the non-contact regime. For samples with different local charge domains ("heterogeneous-charge" samples) the acquisition of electrostatic measurements cannot be performed in jumping or constant frequency (CF- DSFM) on the non-contact regime, because it is not possible to establish a point of feedback since the slope of the interaction curves (normal force and frequency shift) is different for each charge domain (attractive or repulsive) (Fig. 1). However "dissipation", other DSFM channel related to amplitude, is monotonous. Constant amplitude (CA-DSFM) is only way for SFM-images of "heterogeneous-charge" samples.

In this work a lipid bilayer (DOTAP) on mica has been measure in milliQ water. Frequency shift, phase and amplitude channels have been acquired simultaneously with normal force like an additional information channel. Constant amplitude and constant frequency have been compared at low oscillation amplitude in dynamic modes: At constant amplitude good topography has been acquired with right height (6 nm). This mode is reproducible and non-destructive since low forces are applied. At constant frequency wrong height (3.5nm) has been obtained. In addition high forces are applied so this mode is destructive if the measure is instable.

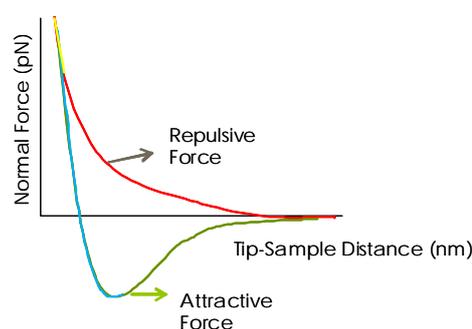


Fig 1. Attractive and repulsive regime in force-distance curves.

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## The interplay between the mechanical properties of viral fibers and the strength of virus-host links during early infection stages

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Viral fibers play a central role in many virus infection mechanisms since they recognize the corresponding host and establish a mechanical link on its surface [1]. Biochemical data indicate that in T4 bacteriophage, at least three of these fibers are required for initial host cell interaction, but do not reveal why three and no other number.

By using Atomic Force Microscopy [2] we obtained high-resolution images of gp37 fibers adsorbed on mica substrate in vitro, and probed their mechanical properties [3]. We hypothesize that three viral fibers provide enough mechanical strength to prevent a T4 virus from being detached from the bacteria by the viral particle Brownian motion.

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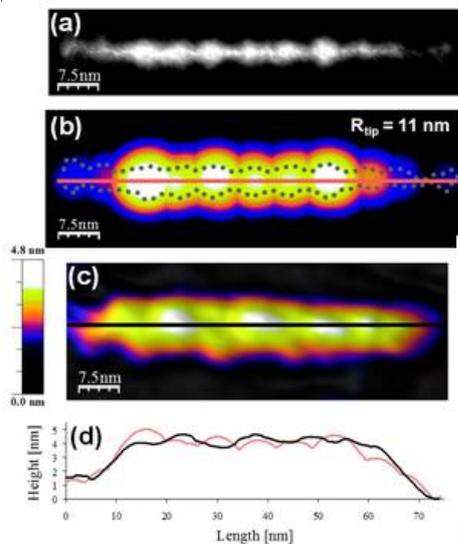


Fig. 1.

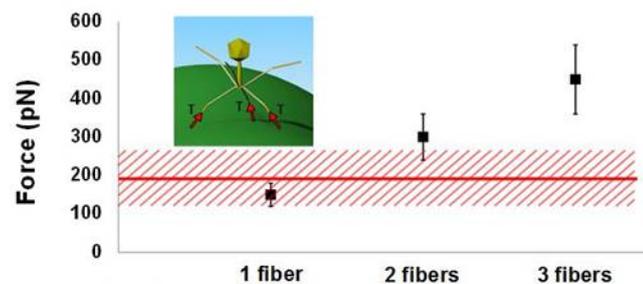


Fig.2.

## Magnetic domain structures in single modulated FeCoCu nanowires

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In this work, we present a Magnetic Force Microscopy (MFM) study on the domain configuration of single FeCo based cylindrical nanowires. FeCo nanowires exhibit the necessary capability to be employed in novel generation of rare-earth-free permanent magnets due to their high Curie temperature, large saturation magnetization and enhanced magnetic hardness [1]. High resolution MFM technique has been used to characterize isolated nanowires deposited onto Si substrates.

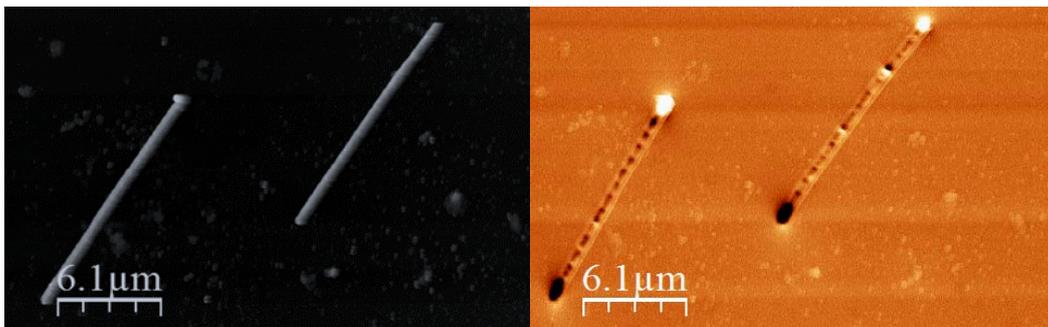
The polycrystalline Fe<sub>28</sub>Co<sub>67</sub>Cu<sub>5</sub> nanowires, growth by electrochemical methods into the anodic alumina membrane, present high shape anisotropy due to their high aspect ratio. Tailoring the membrane pore diameter we can prepare straight nanowires with homogeneous diameter as well as modulated nanowires with diameter varying periodically between 22 nm and 35 nm. MFM imaging allow us to conclude that the straight nanowires posse a dominant single domain behaviour even in the demagnetized state. However, the MFM images corresponding to modulated ones -with increased hardness- show the presence of domain walls.

Micromagnetic simulations [2] predict the magnetization to point along the wire main axis in both cases. Interestingly, in the demagnetized case of modulated wires, simulations predict the existence of two kinds of stable domain walls: single vortex and 180° transversal walls.

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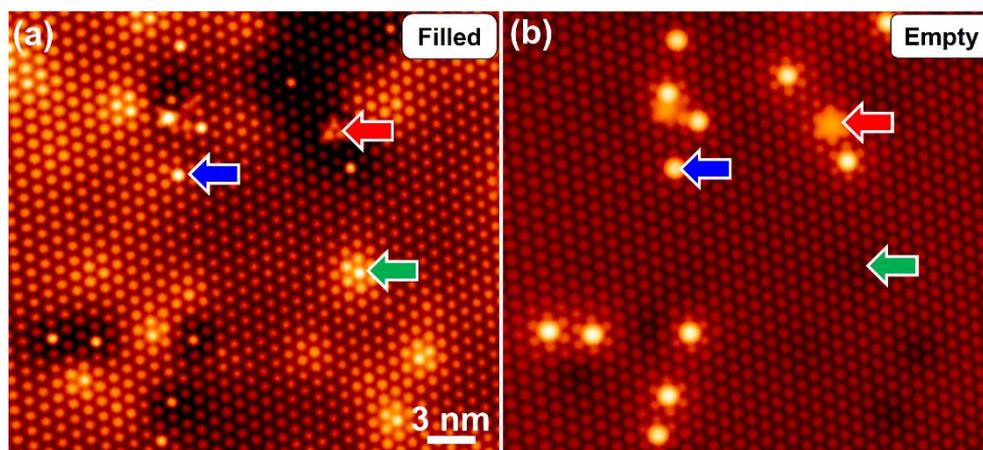
## Investigating subsurface boron dopants in Si(111)-( $\sqrt{3}\times\sqrt{3}$ )R30° using simultaneous nc-AFM/STM and DFT

Jan Berger<sup>1</sup>, Evan J. Spadafora<sup>1</sup>, Pingo Mutombo<sup>1</sup>, Mykola Telychko<sup>1</sup>, Martin Ondráček<sup>1</sup>, Martin Švec<sup>1</sup>, Alastair McLean<sup>2</sup>, and Pavel Jelínek<sup>1</sup>

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B:Si(111)-( $\sqrt{3}\times\sqrt{3}$ )R30° surface has gained a lot of interest in surface science, due to its prominent electronic and structural properties. Compared to bare silicon surface, this system has reduced chemical reactivity, which makes it a suitable candidate for deposition of molecular complexes without a risk of their decomposition. Here, we investigated the near surface defects of this delta-doped system using a combination of scanning tunneling microscopy, non-contact atomic force microscopy, *ab initio* and Green's function theoretical methods. We make positive assignments of two near surface defects: the adatom vacancy and a B substitutional defect that is located in the second Si bilayer. We also confirm the previously reported assignment of the dangling-bond defect. Additionally, the influence of the subsurface defects on the surface electronic structure, in particular the modulation of the surface potential, is investigated using Kelvin probe force microscopy, scanning tunneling spectroscopy and large scale density functional theory calculations. The effects of solitary dopants can play a significant role on commercial device performances as well as on the fundamental local properties of a semiconductor. Therefore, this study paves the way for a deeper understanding of passivated Si surfaces used for the development of molecular thin films and devices.



**Figure 1** STM topographical images of the (a) filled and (b) empty states of the B:Si(111)-( $\sqrt{3}\times\sqrt{3}$ )R30° surface. A Si DB, a subsurface B defect, and a Si adatom vacancy are highlighted by the blue, green, and red arrows, respectively. Image details: 21 nm x 21 nm,  $I_t = 0.5$  nA,  $V_{\text{empty}} = +1.4$  V,  $V_{\text{filled}} = -0.5$  V. Height scale: 0 to 3.5 Å.

## ADSORPTION SITE DEPENDENCE OF VIBRATIONAL EXCITATIONS OF MOLECULAR HYDROGEN

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Transition-metal phthalocyanines are a well-known class of molecules used as model to study the interaction between metal surfaces and metal-organic compounds [1][2]. These kind of metal-organic complexes present a wide range of properties and functionalities which depend on the coordination of their central metal ion, such as magnetism or the adsorption of small gas molecules [3].

In this work we study Chlorinated Manganese Phthalocyanine (Cl-MnPc) molecules deposited on a Ag (111) substrate. We explore the adsorption characteristics of this system by means of a combined Low Temperature Scanning Tunneling and Atomic Force Microscope. After deposition on a room temperature substrate, a fraction of (dechlorinated) MnPc molecules coexist with Cl-MnPc on the surface. Moreover, Cl-MnPc can be controllably dechlorinated after the evaporation process.

We find that both molecules are a preferential site of adsorption for molecular Hydrogen, which is known to present a bistable vibrationally mediated behavior depending on its different adsorption configurations [4]. Inelastic tunneling of electrons from a STM can excite such bistability which induces a fingerprint close to zero-bias on differential conductance measurements. Additionally, force spectra reveal differences on the electrostatic forces exerted between the tip and the molecule when the tunneling electrons trigger such hydrogen fluctuations. We find that these fingerprints are strongly modified by the presence or absence of Chlorine atoms in the phthalocyanine molecules.

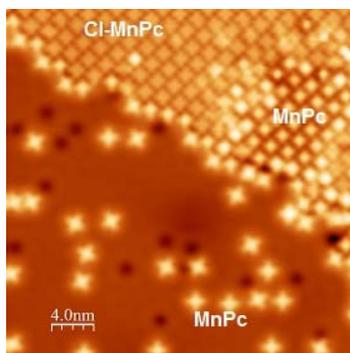
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*Figure 2: STM image of a self assembled island of Cl-MnPc. MnPcs coexist both in the island and in the Ag (111) surface.*

## **Radiation damage evaluation by means of Monte Carlo simulation of atomics displacements processes in Fe, Ge and Si samples.**

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A new algorithm to simulate the stochastic occurrence of atom displacements processes (AD) is developed by the authors. Using the Monte Carlo method, an improved calculation code was done to evaluate the radiation damage produced by gamma and electronic radiation in several solid materials. AD processes were considered only on the basis of single elastic scattering interactions among fast primary and/or secondary electrons with matrix atoms. Taking into account that, AD distributions in sample's depth as well as the energetic profiles of AD events were obtained at different materials (germanium, silicon and iron). Reliable results for both distributions were carried out according to the single elastic scattering cross section proposed by McKinley-Feshbach. Furthermore, a comparison between the primary AD distribution obtained and the theoretical expressions suggested by Oen-Holmes-Cahn is presented and discussed.

## Detecting charging effects of single molecules by nc-AFM

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The ultimate goal in electronic devices miniaturization is the creation of circuit elements (as wires, transistors, rectifiers...) consisting on single molecules. A single molecule transistor exploits the electrostatic modulation of a molecule's orbital energy. To realize such device a high degree of charge localization is needed in order to allow for discrete changes in transconductance of the molecular device [1]. Charge localization requires minimal hybridization between the molecular orbitals and the states of the leads, and the possibility to tune the charge state of the molecule. Scanning probe techniques offer the unique possibility of addressing such issues in studying single molecules with atomic precision. Scanning tunneling microscopy (STM) has proven its potential to discriminate and manipulate the charge state of single atoms and molecules [2]. Non-contact atomic force microscopy (nc-AFM) allowed as well determining the charge state of those systems [3]. Nevertheless the dynamic response of the AFM to (dis)charging events has been investigated so far for many electron systems as semiconducting quantum dots [4] or nanoparticles [5].

Here we demonstrate the capability of nc-AFM to achieve single-electron sensitivity in processes occurring in single molecules. The electron acceptor molecule TCNQ embedded into a charge transfer compound (TCNQ-TMTTF) could be (dis)charged by integers of  $e$  through gating with the electric field between an STM tip and the Au(111) supporting surface [6]. The critical field inducing the molecular (dis)charging could be tuned with the sample bias voltage or the tip-molecule distance. The latter changes periodically at an oscillating AFM tip. The coupling of the (dis)charging process resonantly with the periodic motion of the AFM tip, results on a change of the measured frequency shift ( $\Delta f$ ) due to different electrostatic forces in the junction. By sweeping the applied sample bias,  $\Delta f$  exhibits a pronounced deep whenever the molecule changes from a charged to a neutral state.

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## Atomic Resolution and Moiré Patterns in Graphene/Pt(111) by Low Temperature-NCAFM Experiments and DFT Calculations

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The epitaxial growth of graphene on metals is currently an active field of research [1]. Scanning probe techniques have revealed as fundamental tools for the analysis of the atomic and electronic structure of graphene. However, the origin of atomic contrast in carbon based systems is still a challenging question [2]. Graphene on Pt(111) is of utmost interest due to the low interaction of its pristine surface with the metal [3].

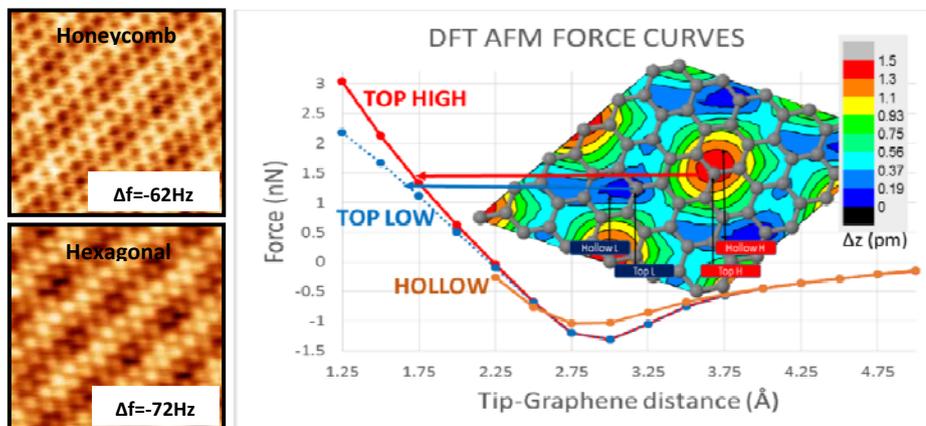
In this work, for the first time, the graphene/Pt(111) system is studied with NCAFM both experimentally and theoretically. With a home-made cantilever-based AFM operating at 5K and UHV, atomic resolution and moiré patterns are observed. Moreover, inversions of atomic contrast from a honeycomb to a hexagonal lattice (with one maximum per unit cell) have been detected. The comparison of experimental specific-site force spectroscopy data with first-principle DFT calculations has allowed gaining further insight. The inversion of atomic contrast may be rationalized in terms of the electronic density dependence of the Pauli interaction [2]. However, we associate the AFM observation of the moiré to sub-surface resolution. According to DFT calculations, corrugated moirés can be obtained in the repulsive regime, where the tip indents the graphene sheet deep enough so the displaced carbon atoms act as a tip that allows sensing the Pt surface with atomic resolution. This idea may be generalized to other 2D materials opening the door to simultaneous monolayer/substrate AFM characterization.

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## High resolution nanomechanical characterization of the early stages of swelling and degradation of biodegradable scaffolds in buffer

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Poly(lactic-co-glycolic acid) (PLGA) is a biocompatible and biodegradable scaffold that is used in many implantable devices. The nanoscale features of the scaffolds, topography and mechanical response, influence the final the device performance. Here we present a high resolution study of the early stages of swelling and degradation of the scaffold upon immersion in a biological buffer. Micrometer-size patterns of PLGA have been fabricated by using focus ion beam lithography. Force microscopy has been used to measure simultaneously the topography, the volume and the elastic response of a single pattern as function of the time immersed in buffer. The nanoscale roughness has a slight increase during the first two days of immersion; this is followed by a continuous descent down to 10% of the initial value. The volume increases until it reaches a maximum at about 8 days. The effective Young modulus shows continuous decrease from an initial value of about 2 GPa down to 9 MPa at day 14. The presence of a maximum in the volume indicates a competition between swelling and degradation. High-resolution images of the PLGA patterns indicate the erosion of the surface.

References:

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Fig.1

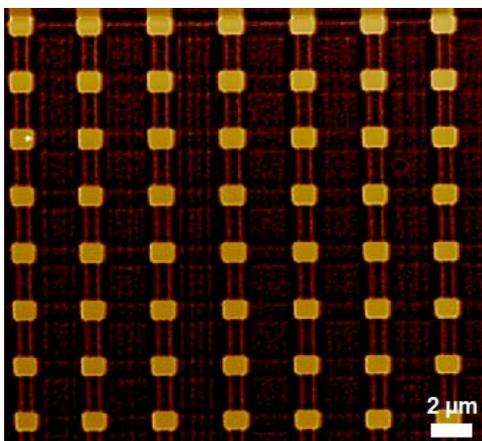
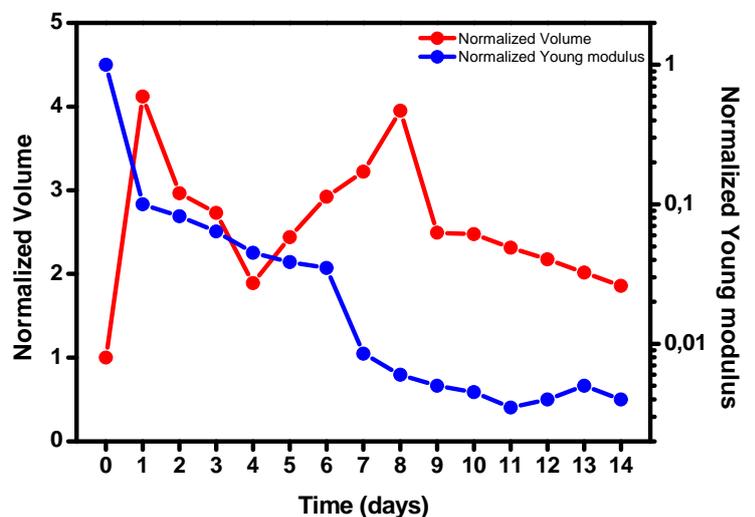


Fig.2



## NCAFM theoretical model for dissipation and Moiré pattern resolution on Graphene on metals

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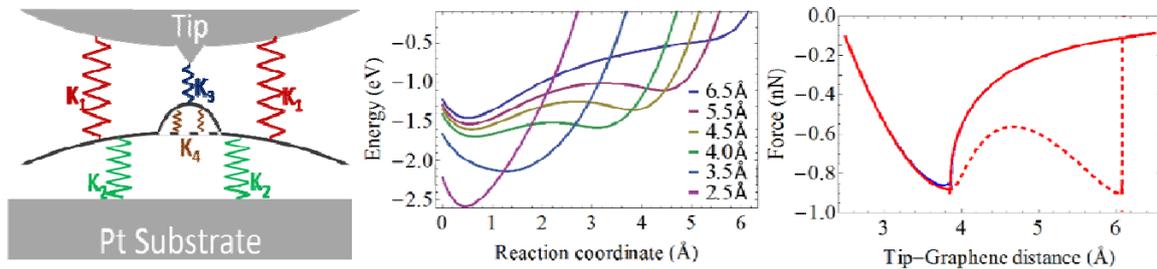
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Because of weak coupling, the observation of the Moiré patterns of Graphene (G) on Pt(111) is a challenging system for the AFM due to the very small topographic corrugations present on the G,  $<2$  pm [1]. However, LT NCAFM measurements of G/Pt(111) is not only able to image the G with atomic contrast but also the modulation of the Moiré patterns. These experiments show the following main characteristic: 1- A plateau of  $\sim 0.8$  eV in the dissipation signal vs distance, 2- atomic and Moiré contrast arise at the same distance than the dissipation, 3- inversion of the atomic corrugation upon tip approach. We use DFT AFM simulations of a  $6 \times 6$  G/Pt cell and a small apex to explain the atomic contrast and contrast inversion of the G [2] and the Moiré modulation in the repulsive regime. However, the limitations in the number of atoms of the DFT method and the lack of a macroscopic tip do not allow for a macroscopic deformation of the graphene needed to explain both the Moiré in the attractive regime and energy dissipations observed in the experiments.

In this work we develop a simple model (see Fig. 1) that allows for local and macroscopic deformations of the G sheet and incorporation of a macroscopic tip-sample interaction using elastic constants determined through DFT. The model predicts a large energy dissipation due to hysteresis of the G deformation: for a finite retraction length, the G sheet adheres to the tip. Furthermore, the model is sensible to small variations of the effective elastic constants arising from subtle differences in the G/Pt interaction, thus explaining the observation of the Moiré in the attractive regime. The same mechanisms are expected to be found on similar AFM experiments on 2D materials [3].



**FIG 1:** Left: Theoretical model with four springs representing: macroscopic/nanoscale tip-graphene interaction and macroscopic/nanoscale deformations. Center: Energy barriers for different tip heights. Right: Predicted forces for two different top sites in a  $3 \times 3$  G moiré.

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## **Investigation of magnetic polymer composites by AFM and MFM techniques**

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Metallic nanoparticles (NPs) have been the matter of significant importance due to their wide variety of applications originating from their unique features such as magnetic properties. Numerous composites have been fabricated by combining the magnetic NPs with polymer which has led to their application in Micro-Electro-Mechanical Systems (MEMS), sensors, etc. Atomic Force Microscopy (AFM) has the ability to demonstrate 3D topographical images of numerous samples made by these NPs incorporated in both synthetic and biopolymers. Furthermore, Magnetic Force Microscopy (MFM) can provide us with magnetic profile of the sample. Therefore, these techniques have been vastly used in wide range of samples one of which is magnetic polymer composite [1]. In this work we have fabricated the magnetic polymer composites with magnetic anisotropy. The proof of the alignment of magnetic NPs in poly(methyl methacrylate) film is acquired through AFM technique which gave us the morphology of the sample. The magnetic data of the magnetic polymer composite was also obtained by MFM with very high nanometer resolution which demonstrated the high magnetic anisotropy of the composites originating from the one-dimensional magnetic alignments in PMMA film.

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## Noise imaging in non-contact Dynamic Scanning Force Microscopy

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Dynamic Scanning Force Microscopy (DSFM) is a very powerful tool for non-invasive imaging of surfaces since extremely low forces are applied on the sample. Most systems are operated in ambient conditions where non-contact DSFM is performed with tip-sample distances of the order of 3-10 nanometers. We will show that the dissipation occurring in ambient conditions within the tip-sample system during NC-DSFM operation leads to significant noise in the tip-sample interaction. To measure noise, the DSFM-system is operated in Amplitude Modulation mode with relatively small oscillation amplitude (about 5- 10nm) and a small amplitude reduction ( $a_{set} \approx 0.95 a_{free}$ ). Noise images are acquired at constant amplitude (amplitude is signal for topography feedback) with a Phase Locked Loop in order to track the resonance frequency and Kelvin Force Microscopy was performed in order to minimize the local electrostatic field between tip and sample. From the noise image we clearly deduce that the noise in the tip-sample system is inhomogeneous and depends on the physical and/or chemical properties of the sample. In addition to the images shown, high resolution local spectroscopy data of the normal force, the noise signal, the amplitude and the frequency shift will be discussed. From the analysis of these curves we find that the noise increases significantly as soon as a reduction of oscillation amplitude is detected. We will discuss whether this significant increase of noise affects resolution of DSFM-related techniques such as Electrostatic and Magnetic Force Microscopy. In addition, we will compare Amplitude Modulation with Frequency Modulation DSFM when operated in ambient conditions.

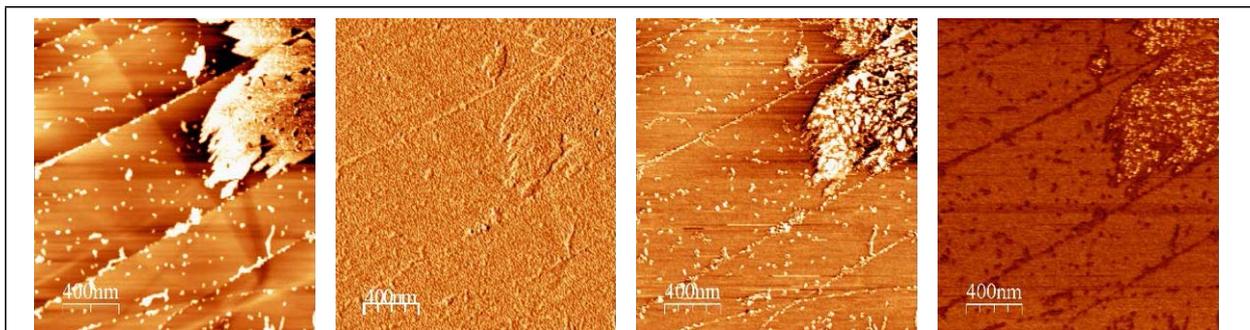


Figure: From left to right, images of topography, frequency shift, co

## Graphene growth on Pt(111) and Au(111) using a MBE solid carbon source

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Graphene is considered a prototype material with interesting technological applications and properties [1]. Preparation methods greatly varies from exfoliation mechanical transfer [2] (widely used in research laboratories), to Chemical Vapor Deposition (CVD) [3] (more appropriate for industrial applications).

In this work, we present a Molecular Beam Epitaxy (MBE) method to obtain graphene [4] on Pt(111). This procedure uses evaporation of carbon atoms from a carbon solid-source in ultra-high vacuum conditions. We have tested the formation of graphene on several surfaces: from a well establish substrate as platinum, to substrates where graphene can be formed using innovative methods as gold [5]. For the characterization of the graphene layers we have used several in situ surface science techniques as LEED, AES and STM.

The successful evaporation of carbon has been probed on different substrates as platinum, HOPG, and gold. By annealing a Pt(111) and Au(111) surfaces up to 600°C and 450°C respectively during carbon evaporation, we have observed a characteristic LEED diagram attributed to graphene [6]. STM images (see figure) display long range ordering of carbon monolayers showing several moirés patterns characteristic of graphene on Pt(111) [7] and islands of dendrites of Au(111) [8], further proving the formation of graphene. This method opens up new possibilities for the formation of graphene on many different substrates with potential technological applications

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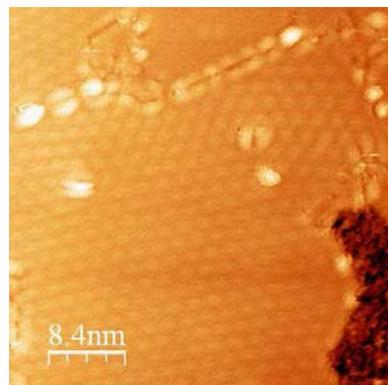


Fig. 1. STM image of graphene on Pt(111) showing long range moirés patterns and atomic resolution (Bias Voltage = -35.7mV, Current set-point = 0.04nA)

## Dissipation in Magnetic Force Microscopy: artifacts or information?

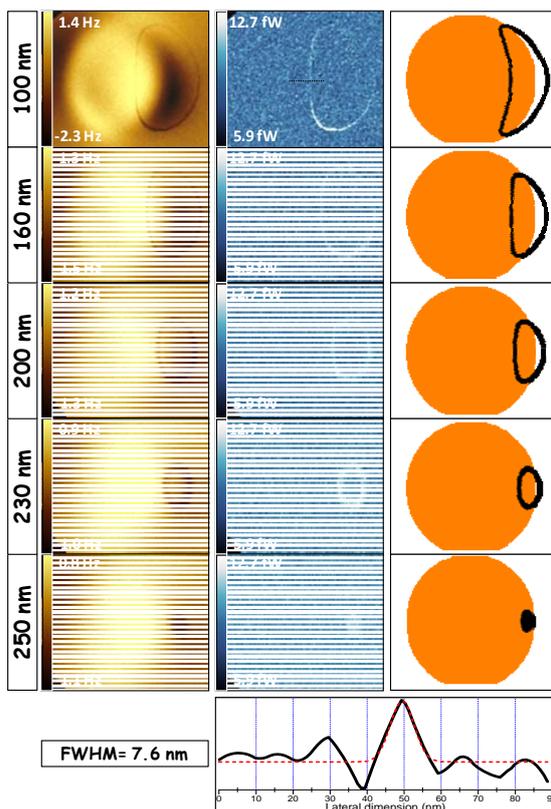
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Measuring dissipation in scanning force microscopy relies on extracting physical information from either tip or sample by recording variations in the cantilever oscillation [1]. Non-conservative interactions between the tip and the sample give rise to a decrease in the oscillation amplitude of the lever, as some energy is transferred in every oscillation cycle into dissipative processes [2].

In this work, we analyze the information extracted from the energy dissipation in Magnetic Force Microscopy [3]. In some cases, dissipation is attributed to rotations of



the magnetization at the tip apex and the subsequent change in the interacting force gradient might be misinterpreted as part of the domain structure of the sample. In the same way, we present a new way of obtaining 3D maps of local magnetic fields at the nanoscale, with a spatial resolution below 10 nm [4]. The figure on the left shows frequency shift and dissipation data (left and central columns) obtained in *Py* circular dots, compared to micromagnetic calculations (right column), for increasing tip-sample distance.

In addition, negative dissipation gradients have been found in materials with strong perpendicular anisotropy (i.e. CoNi multilayer films). Experimental evidence is presented of a counterintuitive monotonous reduction of the dissipation as the tip-sample distance decreases, so that increasing the interaction can result in a

reduction of magnetic losses. The origin of such striking dependence is discussed [5].

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## Intramolecular Dipole of Merocyanine probed by Local Contact Potential Difference

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The merocyanine form of the molecular switch 1,3,3-Trimethylindolino-6'-nitrobenzopyrylospiran exhibits an intramolecular dipole in gas phase and solution [1]. When adsorbed on a metal surface, charge redistribution and screening may considerably alter the expected dipole behavior. Utilizing combined low-temperature scanning tunneling microscope and dynamic atomic force microscope, we characterize the adsorption of merocyanine on metal substrates. The intramolecular charge distribution is measured by the local contact potential difference (LCPD) [2]. The vertical and lateral distribution of the LCPD hints at the persistence of an intramolecular dipole.

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## Precise control of intramolecular H-atom reactions using scanning probe microscopy

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Molecular processes are of fundamental importance in chemistry and their precise control is a key to the future of molecular device applications. Although the atomic-scale environment of a molecule is known to have a significant impact on such processes, local effects have rarely been investigated at the single-molecule level. Recently we reported the direct observation and precise control of intramolecular H-atom transfer reactions, i.e. tautomerization, within a single porphycene molecule adsorbed on a Cu(110) surface using STM [1,2]. Tautomerization is an important elementary processes in chemistry and biology and represents a molecular switch. We demonstrate the direct excitation of the tautomerization within a single porphycene [Fig. 1] and systematic tuning of the tautomerization rate by either placing single Cu adatoms nearby a molecule, or by changing the orientation of neighboring molecules. It is also found that approaching the tip to the molecule can affect the tautomerization and eventually induce the process even without energetic tunneling electrons. Although the interaction between the molecule and atomic-scale surroundings is directly associated with such modifications, the detailed mechanism is still not perfectly understood. Recent advances in NC-AFM technique makes it possible to directly measure forces that drive atomic scale reactions [3,4]. We employ NC-AFM to investigate the interaction between the tip and porphycene molecule, which modifies the potential landscape of the tautomerization.

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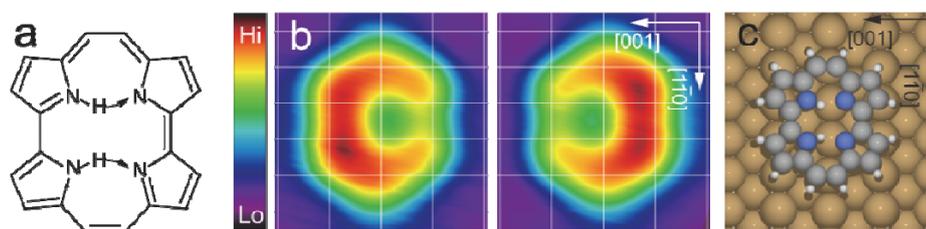


Fig.1. Porphycene molecule on Cu(110). a) Molecular structure (the H-atom transfer during tautomerization is indicated by arrows). b) Typical STM images of a single porphycene on Cu(110) ( $1.49 \times 1.42 \text{ nm}^2$  in size;  $I=10 \text{ nA}$ ;  $V_{\text{tip}}=100 \text{ mV}$ ). The substrate position is indicated by white lines. c) Density functional theory calculated optimized structure.

## Synthesis and Characterization by STM, XPS and DFT of Two Dimensional Covalent Organic Frameworks based on Polyester Condensation

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Understanding the factors that contribute to organization of materials at the nanoscale level is a basic requirement for the development of Nanoscience. In order to obtain such materials, bottom-up strategies focus on the organization of molecules by either non-covalent interactions, leading to supramolecular H-bonded [1] or metal-coordinated assemblies [2,3], or by means of covalent bonds [4,5]. In this work [6] we demonstrate, for the first time, that polyester condensation is a feasible way to achieve the organized assembly of single layers of an unprecedented surface covalent organic framework (SCOF). This SCOF was formed both in bulk scale and under ultrahigh vacuum (UHV) conditions on a Au(111) surface by the reaction of an aromatic alcohol, 1,3,5-tris(4-hydroxyphenyl)benzene (TPB), with an aromatic acyl chloride, benzene-1,3,5-tricarbonyl trichloride (TMC). The characterization performed in situ by means of variable temperature scanning tunneling microscopy (STM) and photoemission spectroscopy (XPS) reveals the formation of an array of hexagonal cavities with ca. 2 nm size. The formation of such structure is further confirmed by density functional theory (DFT) based first principles-calculations. The functionality of ester bridges within the cavities allows to envisage their potential use in molecular recognition processes. Moreover, the judicious choice of adequate building blocks opens the possibility of tuning the structure of the framework, offering a tool to tailoring on demand different levels of porosity.

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## Design an Iterative Learning Observer to Reconstruct the Interaction Force in AM-AFM

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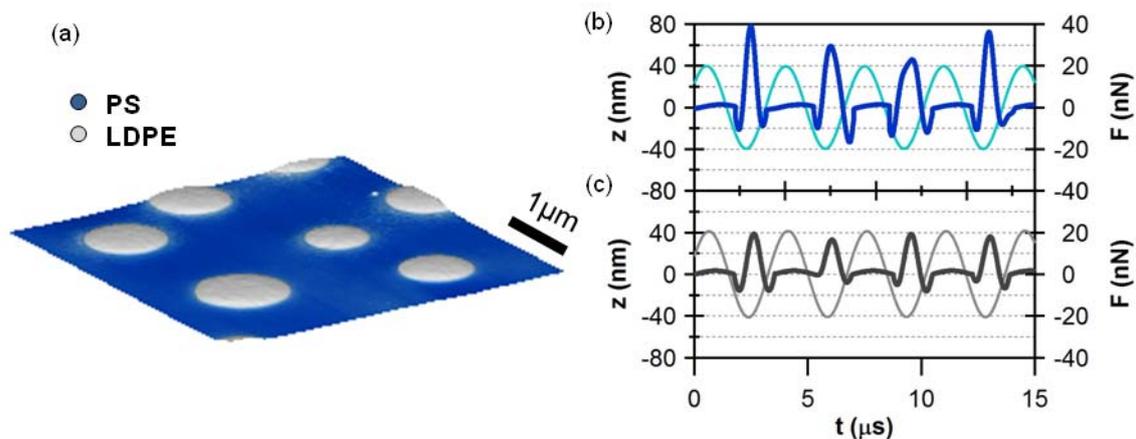
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Extracting the time varying tip-sample interaction force in dynamic atomic force microscopy has been an important goal to improve the imaging capabilities of AFM with simultaneous measurements of material properties [1-4]. Here, we design an Iterative Learning Observer to reconstruct the interaction force from the wave profile of the cantilever. In this method, the interaction force is considered as an unknown time varying parameter and estimated by the designed observer.

Simulations and experiments prove the accuracy of this method in liquid and air for different materials. From the reconstructed force signals, we are able to obtain the average peak force, and consequently, using Hu and Raman equation [5], the Young modulus of the materials.

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(a) Topography image of Polystyrene (PS) and Polyolefin Elastomer (LDPE) blend. (b) Signal and reconstructed force of PS ( $A_0=78\text{nm}$ ) (c) Signal and reconstructed force of LDPE ( $A_0=78\text{nm}$ ).

## STM and nc-AFM investigation of submonolayer copper oxide structures

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With the aim of obtaining laterally heterogeneous surfaces with catalytic properties, submonolayer coverages of ultrathin copper oxides on Cu(111) have been grown by air injection and annealing in UHV [1-3] and investigated by means of STM/nc-AFM. Different oxide surface structures have been observed depending on the stoichiometric oxygen/copper ratio, some of which have been already reported [1, 2]. In addition, a new open honeycomb structure with a relatively large unit cell lattice parameter of  $\sim 1.3$  nm has been observed that nucleates and grows at the step edges of the oxide terraces. This oxide structure can be visualized as an ordered surface network which might serve as nanopattern template for controlled molecular organization (i.e. in a bottom-up approach). Moreover, derived from the expected semiconducting character of the oxide, the ultrathin layer would offer as well an effective electronic decoupling of the organic molecules from the metal surface.

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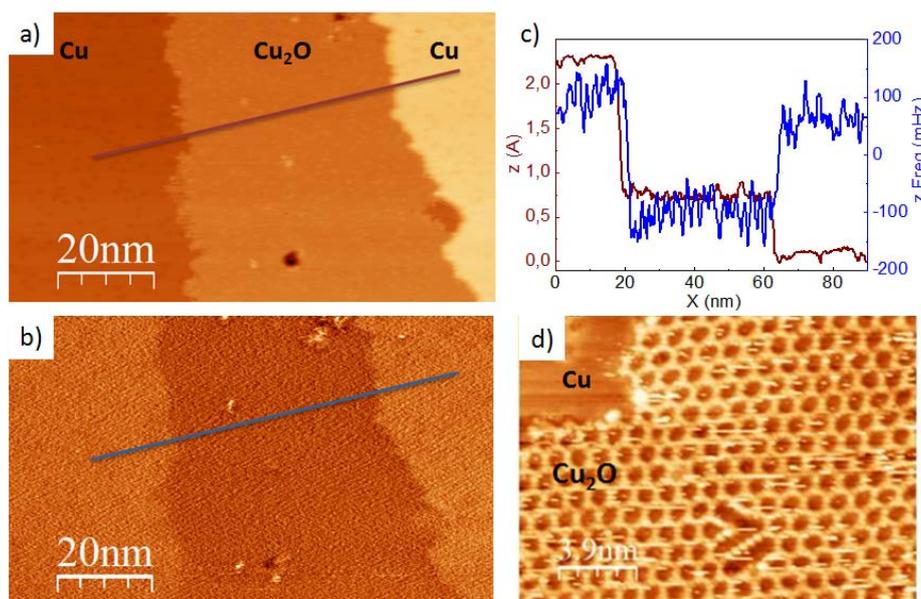


Fig. 1: a) Dynamic STM image of a copper oxide in the ledge of a monoatomic copper step, b) the corresponding frequency channel and c) the topographic line profile of images a) and b), respectively. d) Dynamic STM image of the open herringbone structure with lattice parameter of  $\sim 1.3$  nm.

## Imaging differences in local electronic structure with $\kappa$

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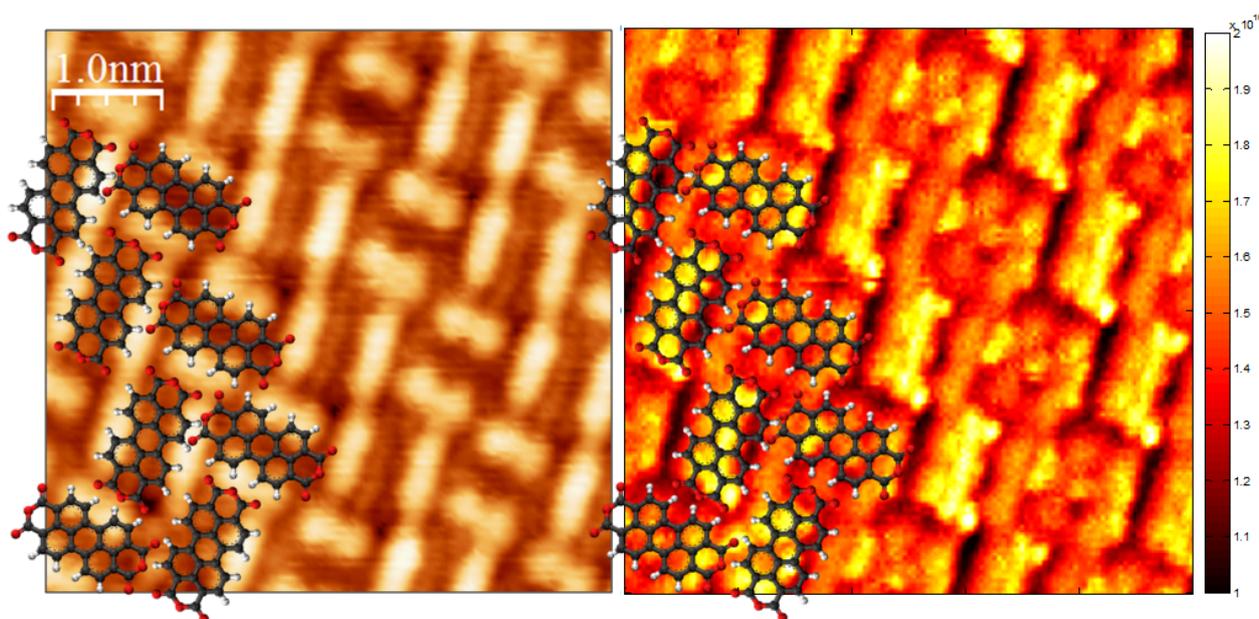
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Performing AFM with a conducting tip allows the electronic structure of the surface to be investigated. The most common technique is Kelvin Probe Force Microscopy. However, with this technique, simultaneous STM is difficult, because of the varying bias potential. We propose an alternate technique [1], first introduced by the STM community [2], in which measurements of the tunnel current at the oscillating frequency of the tip can yield information about the vertical decay constant of the tunneling current,  $\kappa$ . This permits a measure of the electronic structure at room temperature as well as combined STM/AFM.

We have studied the electronic structure of PTCDA islands on Ag/Si(111)-( $\sqrt{3}\times\sqrt{3}$ ). In the herringbone structure, two non-equivalent adsorption sites exist, in normal AFM these differences are hard to detect [3] however we are able to detect in the  $\kappa$  map.

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**Figure:** STM topography (left) and  $\kappa$  channel (right) of a PTCDA herringbone island

## **Towards a new bio-quantum model for signaling and repair of DNA damage**

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The mechanisms by which eukaryotic cells perceive and recognize breaks in DNA strands have not yet been elucidated. The rapid induction of ATM kinase activity immediately after exposure to ionizing radiation suggests that radiation acts at a previous stage of signal transduction. Former studies suggest that activation of ATM does not need a direct link with DNA strands damages (ATM is located outside the nucleus). But some questions remained open, as for example, how the ATM perceives the break? How proteins like ATM respond coordinately recognizing several DNA double strand breaks (DSB) inserted in a universe of 3 billion base pairs? Which factors determine the high response rate and extent of the ATM? In this work we propose an original model for the signaling mechanism of the ATM kinase, as well as for the recognition of DSBs embedded in a genome of billions of base pairs. It is envisaged that this also could give satisfactory answers to some of the key issues mentioned above. It will be proposed and worked out a model for signaling between DNA and repair proteins, based upon already established concepts related to the existence of solitons in macromolecules and cells. It will be incorporated to the model a quantum-coherent effect known as free water dipole laser, which is expected to explain how the ATM (a "molecular motor") delineates its navigation route toward the DNA damaged site. Preliminary experimental evidences obtained by our group, as the likely electric character of DNA-repair mechanism, will be reinterpreted.

## Surface phase transition driven by deprotonation reaction

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Molecular self-assembly on surfaces is of great interest due to large number of applications such as catalysis [1] and fabrication of new functional materials [2,3]. Up to now, a great effort has been given mainly to metallic surfaces [4,5], while comparatively little is known about molecule-surface interaction and chemical reactivity of organic molecules on insulating surfaces. However, for many applications such as molecular electronics, phase-supported organic catalysis or molecular optics, the replacement of metallic materials with insulators may improve the performance of such devices or be even crucial in some cases (e.g. to eliminate leaking currents).

In collaboration with the experimental group of Prof. A. Kuhnle at Mainz University, we aim to understand the reactivity of 2,5-dihydroxybenzoic acid (DHBA), an organic molecule deposited on a insulating substrate of calcite. Non-contact AFM experiments show that DHBA molecules deposited at room temperature initially form two different molecular structures: (i) a striped phase, which consists of hydrogen-bonded molecular dimers and (ii) a dense, highly packed phase of de-hydrogenated molecules covalently bonded to the calcite surface. Interestingly, after several hours of observation the striped phase gradually transforms into the dense one, which then remains the only one present [6]. We have investigated this phase transition by performing ab-initio calculations in conjunction with kinetics modelling. In particular, we have studied the adsorption configurations, diffusion and de-hydrogenation mechanisms of a monomer on the surface.

In the present communication, we will show our recent results and compare them with the experimental measurements.

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## Temperature Dependent Electron Transport Properties of Goldnanoparticles and composites: Scanning Tunneling Spectroscopy Investigations

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The importance of catalytic activity of goldnanoparticles (AuNPs) for industry relevant applications has initiated several new research perspectives [1]. AuNPs has emerged as a potential candidate for verity of applications when combined with polymers [2]. Sumati et.al [3] has talked about the charge storage properties of AuNPs and it's composite with urethane-methacrylate comb polymer (UMCP). So it is worth to examine AuNPs and its composites with UMCP to make further comment on their electron transport mechanism. In the current study STS is used for investigating variations in electronic properties of AuNPs and its composite with UMCP as a function of temperature. Films are prepared by drop casting AuNPs and UMCP in a desired manner on silicon substrates. In total four samples are prepared by changing the deposition order of AuNPs and UMCP as well as by modifying the synthesis procedure of AuNPs. Samples are further analyzed for morphology under scanning electron microscopy and atomic force microscopy. STS measurements are performed in the temperature range of 33 to 142<sup>o</sup> C with the help of home made heater, calibrated by standard PT100. Systematic variation in current versus voltage (I-V) curves exhibiting semiconducting to metallic transition/ Schottky behavior is observed for different samples, depending upon the preparation method and as a function of temperature. During the current versus time (I-t) measurement for AuNPs, random telegraphic noise is observed at room temperature. Random switching of tunneling current between two discrete levels is observed for this sample. Power spectra derived from I-t shows  $1/f$  dependence. Statistical analysis of the fluctuations shows exponential behavior with time width  $\tau \approx 7$  ms. Local density of states (LDOS) plots derived from I-V cures of each sample, shows systematic shift in the valance/conduction band edge towards/away from Fermi level, with respect to increase in temperature. Schottky emission is found to be the best fitted electron emission mechanism for all samples over certain range of bias voltage. Schottky plots are used to calculate barrier heights for all samples. Temperature dependent measurements helped in measuring activation energies for all samples. Arrhenius plots shade light on the amount of activation energies involved for classical hopping transport of individual charges between the nearest neighboring particles. Thus variation in electronic properties for all samples as a function of sample temperature are thoroughly examined.

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## Fast Nanomechanical Spectroscopy of Soft Matter

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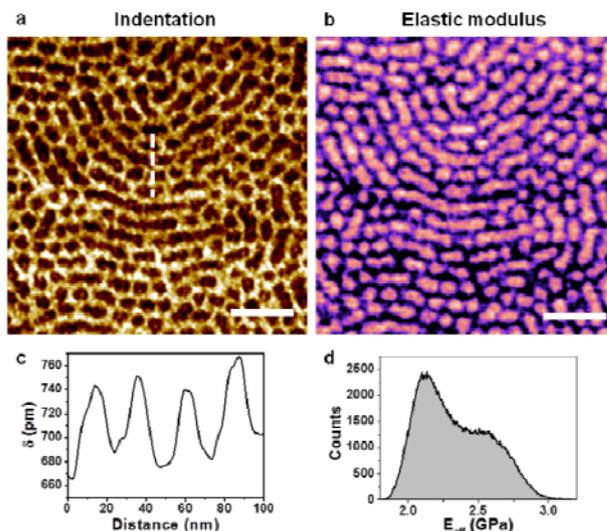
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A method that combines high spatial resolution, quantitative and non-destructive mapping of surfaces and interfaces is a long standing goal in nanoscale microscopy. The method would facilitate the development of hybrid devices and materials made up of nanostructures of different properties.

Bimodal atomic force microscopy is a multifrequency dynamic force method based on the simultaneous excitation of two eigenmodes of the cantilever [1,2]. We have developed a multifrequency force microscopy method that enables the simultaneous mapping of the nanomechanical spectra of soft matter surfaces with nanoscale spatial resolution [3,4]. The properties include the Young modulus and the viscous or damping coefficients. In addition, it provides the peak force and the indentation. The method has been tested on different polymers and proteins in air with near four orders of the magnitude variations in the elastic modulus, from 1 MPa to 3 GPa. The method does not limit the data acquisition speed or the spatial resolution of the force microscope. It is non-invasive and minimizes the influence of the tip radius on the measurements. The use of several information channels (first and second mode) results in the calculation of Young modulus and viscosity coefficients which do not depend on the applied force. The results coincide with the results obtained by other well-established methods (static AFM, force inversion methods).

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**Figure 1.** (a) Indentation map in a block copolymer (PS-b-PMMA) thin film (scale bar, 100 nm). (b) Map of the elastic modulus of PS-b-PMMA (scale bar, 100 nm). (c) Cross-section along the dashed line shown in a. (d) Histogram of the elastic modulus obtained from b.

## Finer features of radiologic effects induced by ionizing radiation

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All cells host long chained molecules. DNA, among them, is the longest and more important, once it is structured into base-pairs codifying genetic information and responsible for the whole dynamics inside the cell. The interaction of ionizing radiation with biological material produces many types of damages at the cellular level, particularly in DNA, the largest radiation target [1]. The commonly accepted model assumes DNA breakage taking place randomly all along the strands [2]. However, recent studies carried out by this group in this Laboratory, using high-resolution Atomic Force Microscopy and linearized plasmid DNA, came out with quite unexpected results. From these, it was found out that while electron beams severely shatter the DNA strands, into myriads of pieces, the fragment distributions from irradiation with low energy (1.6 MeV) gammas presented discrete-like patterns at all doses, suggesting that these patterns are modulated by the base pair composition of the plasmid. These findings raised a so far unanswered question: *Why the DNA fragmentation patterns are so distinct when induced by gammas and electrons, since these two radiations have comparative LETs (linear energy transfer)?* This issue was tentatively addressed by arguing that secondary electrons [3] are at least one order of magnitude more intense when produced by electrons comparatively to gammas [previous work from this Laboratory]. It is here proposed the widening of this subject in order to delineate, theoretically and experimentally, the main and finer features of radiologic effects induced by ionizing radiation as distinct as gammas, electrons, alpha particles, neutrons and protons. Instead of plasmid DNA, it will be used in this case cell cultures. The methodology will be constituted by cellular and molecular techniques with Pulsed Field Gel Electrophoresis and Atomic Force Microscopy, respectively. It is intended, therefore, to establish a cause-effect link between cellular viability and genomic DNA fragmentation pattern, toward a better understanding of DNA repair performance. It is expected, as a by-product, to contribute with insights for prevention and therapy of diseases associated with DNA damage and mutation, as e.g. cancer and Alzheimer.

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## DFT study of AFM metal oxide imaging modes: towards atomic species identification

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Metal oxides have many diverse technological applications in fields ranging from catalysis to electronics. Scanning probe microscopies have proven their extraordinary capacity in characterizing the surface properties that govern the chemical and electrical response of metal oxides at the atomic scale.

Here we present a joint study on the Cu(110)-(2x1)O surface [1,2], where the oxide features added rows of alternate copper and oxygen atoms atop the metal surface (Fig. 1A). Atomic force microscopy (AFM) images of the metal oxide show stripes with bright and dark spots (Fig. 1B) but it is not possible to distinguish between species in the added row. Density functional theory (DFT) calculations were performed with two different tip terminations consisting of single copper and oxygen atoms. The strength of the interaction of the tip with the added row was measured following a previously reported protocol [3] for the simulation of the AFM experiments.

While surface reactivity is different for each tip termination, (Fig. 1C) we can conclude that maxima in the AFM images correspond to copper atoms in the added row.

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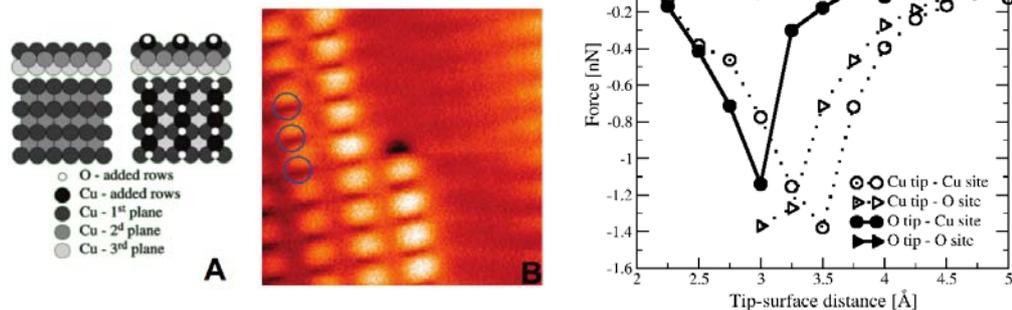


Fig. 1. (A) Side and top view of metal-only (left) and metal oxide (right) of Cu(110)-(2x1)O surface [2]. (B) AFM image showing metal oxide domain (left) and metal-only domain (right). (C) Theoretical force spectroscopy curves obtained from DFT simulations

## A Theoretical DFT Study of Unusual Moiré Patterns in the Graphene/Rh(111) System

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The growth of graphene on transition metals by means of different procedures has been highly studied in recent years [1]. These interactions do not only change the electronic properties of graphene, but also its geometrical structure, leading in some cases to periodic Moiré superlattices. It has been shown, if the graphene-metal interactions are low enough, that several Moiré structures in the system with different sizes may be present [2]. In the case of the graphene on Rh(111), in which interactions are not considered low [1], it has been found a Moiré structure (aligned 11x11 Rh(111) and 12x12 in grapheme) [3,4]. This Moiré pattern has been well characterized by experimental techniques (LEED and UHV-STM) [3] and with ab initio DFT calculations [4].

In this work, we report the existence of different smaller Moiré patterns in the system graphene/Rh(111) by VT-STM experiments. These structures are stable and similar to the one obtained before. The main difference of these structures is that apparent corrugation seems to increase according to the unit cell size of the Moiré pattern. To go in depth in the understanding of the interactions between graphene and rhodium in this system we carry out a series of DFT simulations in some of these new structures. In order to compare them with experimental results we calculate the theoretical STM images based on the Tersoff-Hamann approximation (fig. 1).

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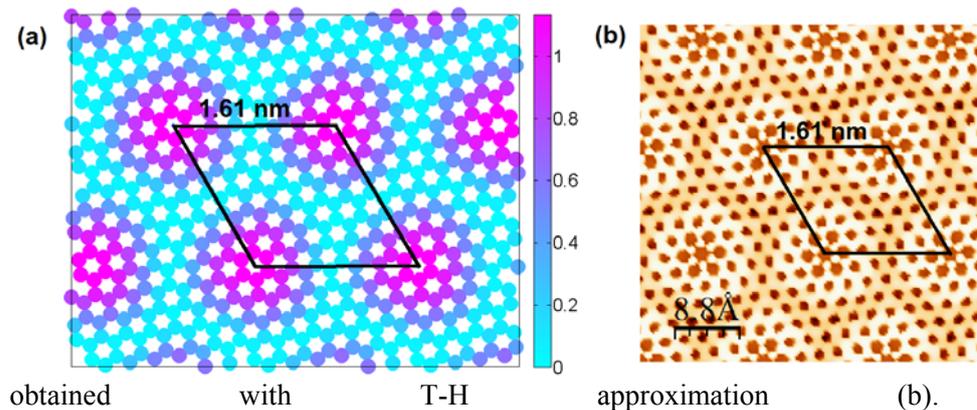
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Fig. 1. Height map (in Å) of one Moiré pattern (6x6 in Rh(111) and  $\sqrt{43}\times\sqrt{43}$ -R7.6° in grapheme) (a) and theoretical STM images of this system



**Artifacts in combined STM/AFM due to non-ideal ground in an STM pre-amplifier**

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In AFM, it is normal to apply a bias voltage between the tip and the sample, most often to compensate for the contact potential difference. In order to perform simultaneous STM, the tunneling current must be measured. This usually involves a preamplifier that holds its current input terminal at a virtual ground that is ideally equal to real ground. Limitations of amplifier bandwidth, gain and slew rate lead to time-dependent deviations of virtual ground from zero, causing a time-dependent variation of the electrostatic force between tip and sample. These time-dependent deviations can lead to artifacts in apparent dissipation and even to an apparent "self" excitation of the cantilever. Here, we monitor virtual ground and discuss the effect of virtual ground deviations to apparent dissipation.

## Characterization of trimethylammonium-based ionic liquid surfaces with Scanning Force Microscopy

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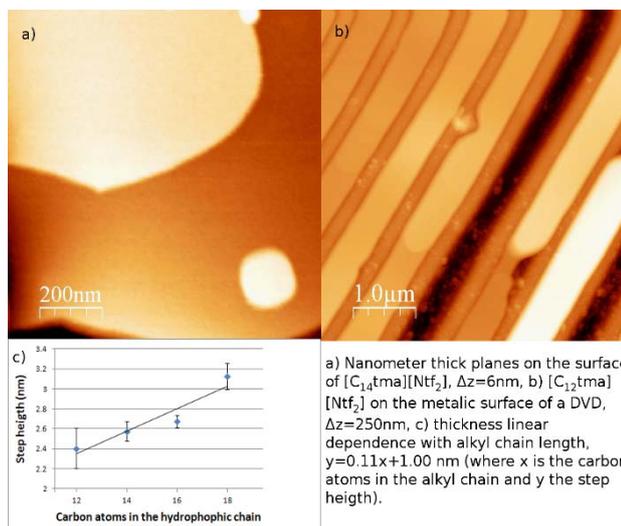
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The objective of this work is to investigate the superficial structure of an ionic liquid family widely used in various fields of science to better understand the unique properties of these molten salts and their modern applications: energy storage devices, lubricants or solvents for nanoparticle stabilization, materials extraction or reactive catalytic supports [1] among other uses. For this study we have used hydrophobic ionic liquids (ILs) based on trimethylammonium cations with long alkyl side-chains,  $[C_n\text{tma}][\text{Ntf}_2]$ , with  $n=12, 14, 16$  and  $18$ , on top of a metallic substrate.

For the nano-characterization of the surfaces we have used a Scanning Force Microscope working in the dynamic mode, finding large flat planes of nanometer thickness for all samples prepared indicating nanocrystalline ordering [2], [3]. Thickness dependence with alkyl side-chain length has been also studied in detail in these compounds [4]. When these ILs are deposited on a structured substrate (e.g. the metallic covering of a DVD) they fill up the tracks on the DVD and grow above them without flooding the available surface. The upper surface of these IL walls stay flat and exhibit a rich dynamics as shown in the pictures.



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## Electron scattering of Rashba-split states in the $\text{BiAg}_2$ surface alloy

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Spin-orbit interaction (SOI) in metallic surfaces can lead, via the Rashba effect, to a splitting of the spin degeneracy and the emergence of particular spin textures that are related to the entanglement between spin and orbital momentum.

Here we use the  $\text{BiAg}_2$  surface alloy, which is characterized by the strongest to date Rashba effect [1,2], to study the effect of SOI on scattering. The alloy is formed on the  $\text{Ag}(111)$  surface after the deposition of  $1/3$  monolayer of Bismuth, which induces a  $(\sqrt{3} \times \sqrt{3})R30^\circ$  reconstruction. The scattering has been studied using Scanning Tunnelling Microscopy and Spectroscopy (STM/STS). In this way we have studied electron confinement by measuring the interference patterns formed by surface electrons scattered from monoatomic steps. We find that scattering is determined by i) an unconventional orbital/spin texture of the surface bands, which give rise to transitions with combined orbital and spin flips, and ii) by its chemical composition, which defines a heterogeneous electron localization and potential landscape. The negligible leakage we observe across some step structures indicate a strong confinement effect, comparable to that observed in metals with marginal SOI such as  $\text{Ag}(111)$  [3]. The results describe a scenario that is far more complex than the conventional Rashba-type two dimensional free-electron gas.

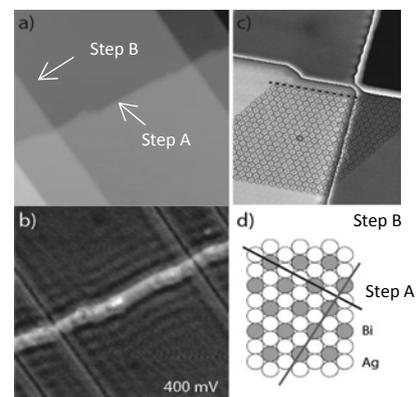
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Fig. 3: (a) Topographic image of a zone of the sample with different type of monoatomical step, acquired with  $I_t = 0.59 \text{ nA}$  and  $V_{bias} = 0.2 \text{ V}$ . Image size:

$400 \times 400 \text{ \AA}^2$ . (b)  $dI/dV$ -map acquired at  $V_{bias} = 10.4 \text{ V}$ . Note that the intensity of the standing wave scattered from the two kind of steps is different. (c) Topographic image performed with

$I_t = 0.59 \text{ nA}$ ,  $V_{bias} = 28 \text{ mV}$ . Image size:  $164 \times 110 \text{ \AA}^2$ . The surface lattice structure is resolved in the image, and the different termination of each step



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## **High-quality single atom N-doping of graphene/SiC(0001) by ion implantation**

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We report a straightforward method to produce high-quality nitrogen doped graphene on SiC using direct nitrogen ion implantation and subsequent stabilization at temperatures above 1300K. In addition, we demonstrate that double defects, which comprise two nitrogen defects in a second-nearest-neighbor (meta) configuration, can be formed in controlled way by adjusting the time of bombardment. We also explain atomic STM contrast of single N-dopants in terms of the quantum interference, which provides more information about electron transport in the N-doped graphene.

## NC-AFM assisted DFT investigation of attachment and chemical reactivity of pentacene molecules on the (101) surface of TiO<sub>2</sub> anatase

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Promising candidates for future organic solar cell and transistor devices include complex nanoscale structures, with thin films of organic molecules and metal oxides layered between metallic electrodes. Optoelectronic activity combined with high charge carrier mobility of conjugated pentacene molecules and the TiO<sub>2</sub> anatase polymorph identifies them as valuable materials for device components [1, 2].

We turn to first-principles simulation techniques in combination with NC-AFM/STM imaging and characterisation of pentacene molecules on the (101) surface of TiO<sub>2</sub> anatase to gain insight into how these materials interact. Aided by experimental images, we identified the preferential attachment site and geometry for adsorbed pentacene molecules. Electronic structure analysis of this organic/inorganic interface showed that molecular orbitals of pentacene introduce localised electronic states into the band gap of the TiO<sub>2</sub> anatase substrate, which may be exploited for optoelectronic functionality in devices. NC-AFM images of adsorbed pentacene molecules reveal intramolecular structure [Fig. 1A]. We employed small TiO<sub>2</sub> clusters with a hydroxyl chemical termination as probe models [3] to simulate AFM experiments over pentacene molecules [Fig. 1B] in order to characterise the contrast formation mechanisms behind the high-resolution imaging and explore system chemistry.

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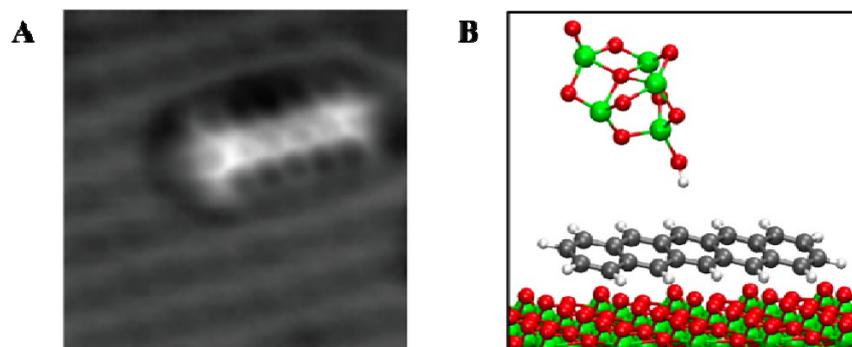


Fig. 1. A. NC-AFM image of a pentacene molecule adsorbed to the (101) surface of TiO<sub>2</sub> anatase. B. Atomistic model employed in DFT simulations of the corresponding experiment

## Quantifying Molecular Stiffness and Interaction with Lateral Force Microscopy

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The spatial resolution of non-contact atomic force microscopy (AFM) can be drastically increased by terminating the tip with a single CO molecule: Images of molecules appear similar to well-known ball and stick models [1]. However, the CO molecule is not stiff and lateral forces, such as those around the sides of molecules, distort images [2]. This begs a larger question: How can an AFM probe structures that are laterally weak? We combined AFM and lateral force microscopy (LFM), both in the frequency-modulation mode, to investigate a CO molecule with a CO-terminated tip [3]. Not only can LFM be used to investigate laterally-weak adsorbates, it measures lateral stiffnesses that are not accessible to AFM. With LFM, we determined the torsional spring constant of the CO molecule on the tip to be 0.24 N/m. This value is less than that of a CO molecule on a Cu(111) surface and an example of a system whose stiffness is a product not only of bonding partners but also local environment.

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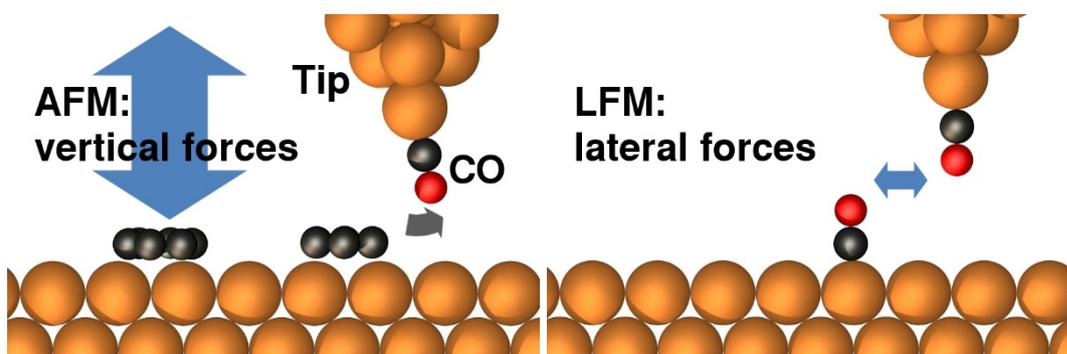


Fig. 1. Normal-mode AFM is sensitive to both short- and long-range interactions.

Fig.2. LFM is sensitive to only short-range interactions.



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## THE ORGANIZERS

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## XXI International Summer School "Nicolás Cabrera"

NEW FRONTIERS IN SCANNING FORCE MICROSCOPY: FROM  
ULTRAHIGH-VACUUM TO BIOLOGICAL MATERIAL

Madrid, Spain, 14-18 July 2014

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***ORGANIZER: José María Gómez-Rodríguez***  
***Universidad Autónoma de Madrid (Spain)***



José María Gómez-Rodríguez obtained his PhD in Physics in Madrid in 1992, under the supervision of Prof. A.M. Baró, with a thesis entitled "Conventional and Fractal Geometries on Microfabricated Samples: a Scanning Tunneling Microscopy Study". After a post-doctoral research stay in the CNRS in Grenoble (France), he came back to Spain and obtained a permanent position at Universidad Autónoma de Madrid (Spain). Since 2000, he leads the research group NanoSPM at the Department of Condensed Matter Physics, Universidad Autónoma de Madrid, in the fields of Nanoscience, Nanotechnology and Scanning Probe Microscopies (SPM). Five major lines have centered his research activity in the last years: 1) Growth and electronic structure of graphene; 2) Thermal stability of atoms, molecules or small aggregates adsorbed on surfaces (surface diffusion and dynamical processes); 3) Phase transitions and critical phenomena on surfaces; 4) Organic-inorganic interfaces (self-assembly and electronic properties of molecular layers adsorbed on surfaces); and 5) Major instrumentation developments in scanning probe microscopies. In particular, he has pioneered in Spain the design and construction of several scanning tunneling microscopes operating under ultra-high vacuum (UHV) conditions as the first spanish UHV variable temperature scanning tunneling microscope (STM), the first spanish UHV low temperature (4K) STM, and the first spanish UHV low temperature (4K) noncontact atomic force microscope (NC-AFM). He is co-author of the third highest cited paper in all the history of his Institution, the Universidad Autónoma de Madrid. He is co-author of WSxM -one of the most used softwares for scanning probe microscopy all over the world- and he is cofounder of the spin-off company Nanotec Electrónica S.L., the only Spanish company devoted to the design and fabrication of scanning probe microscopes.

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***ORGANIZER: Rubén Pérez***

***Universidad Autónoma de Madrid (Spain)***



Ruben Perez graduated in Theoretical Physics in the Universidad Complutense de Madrid in 1987 and got his Ph.D. from Universidad Autonoma de Madrid (UAM) in 1992. After a three-year postdoctoral stay at the Cavendish Laboratory, University of Cambridge, as a Marie Curie Fellow and Research Associate, he returned to the UAM, where he is now a Full Professor of Condensed Matter Physics and leader of the Scanning Probe Microscopy Theory and Nanomechanics Group.

His research has focused on the quantum mechanical modeling of different problems in Materials Science and Nanotechnology that involve forces and currents at the atomic scale, working in close collaboration with experimental groups worldwide. His group ([www.uam.es/spmth](http://www.uam.es/spmth)) has pioneered the theoretical analysis and contrast interpretation of probe-based experimental techniques such as scanning tunneling microscopy (STM) and atomic force microscopy (AFM). His activity has recently expanded into two new topics: the study of oxide materials for catalysis and energy applications, and the AFM characterization of large biomolecules and the structure of self-assembled monolayers in their native liquid environment.

Ruben has co-authored more than 115 publications in international peer-review journals, including Nature and Science, and given 49 invited talks at international conferences. He has been the chairman or member of the Programme and Advisory Committees in more than 20 international conferences and workshops, and belongs to the Steering Committee of the Non-contact AFM Conference since 2005. He has performed stays as invited researcher at different international institutions including the Joint Research Center for Atom Technology (Tsukuba, Japan), the Max Planck Institut für Metallforschung (Stuttgart, Germany), the Fritz-Haber-Institute der MPG (Berlin, Germany) and the National Institute for Materials Science (Tsukuba, Japan); and he has been Visiting Professor in the Osaka University (Osaka, Japan, 2001) and the Lawrence Berkeley National Laboratory (Berkeley, USA, 2012).

Timetable	Monday 14 July	Tuesday 15 July	Wednesday 16 July	Thursday 17 July	Friday 18 July
8:30-9:00	<b>Opening</b>				
9:00-9:50	<b>Franz Giessibl</b>	<b>Hirofumi Yamada</b>	<b>Jose Ignacio Pascual</b>	<b>Ernst Meyer</b>	<b>Ernst Meyer</b>
9:50-10:40	<b>Suzanne Jarvis</b>	<b>Leo Gross</b>	<b>Suzanne Jarvis</b>	<b>Hirofumi Yamada</b>	<b>Leo Gross</b>
10:40-11:20	<i>Coffee break</i>	<i>Coffee break</i>	<i>Coffee break</i>	<i>Coffee break</i>	<i>Coffee break (10:40-11:00)</i>
11:20-12:10	<b>Oscar Custance</b>	<b>Michael Crommie</b>	<b>Oscar Custance</b>	<b>Michael Crommie</b>	<b>Ricardo Garcia</b> (11:00-11:50)
12:10-13:00	<b>Alexander Schwarz</b>	<b>Peter Grutter</b>	<b>Takeshi Fukuma</b>	<b>Alexander Schwarz</b>	<b>Udo Schwarz</b> (11:50-12:40)
13:00-14:00	<i>Lunch</i>	<i>Lunch</i>	<i>Lunch</i>	<i>Lunch</i>	<b>Poster awards.Closing</b>
14:00-15:00					<b>remarks (12:40-13:00)</b>
15:00-15:50	<b>Franz Giessibl</b>	<b>Ricardo Garcia</b>	<b>Udo Schwarz</b>	<b>Adam Foster</b>	<i>Lunch</i>
15:50-16:20	<b>Adam Foster</b>	<b>Stephen Jesse</b>	<b>Pedro J. de Pablo</b>	<b>Stephen Jesse</b>	<b>BUS TO BARAJAS</b>
16:20-16:40			<b>Agustina Asenjo</b> (16:20-16:50)		<b>AIRPORT</b>
16:40-17:10	<i>Coffee break</i>	<i>Coffee break</i>	<i>Coffee break</i>	<i>Coffee break</i>	
17:10-18:00	<b>Takeshi Fukuma</b>	<b>Jose Ignacio Pascual</b>	<i>Visit to the city of</i> <b>SEGOVIA</b>	<b>Peter Grutter</b>	
18:00-19:00	<b>Poster Session</b>	<b>Poster Session</b>		<b>Poster Session</b>	
19:00-20:00	<i>Free Time</i>	<i>Free Time</i>	<i>Dinner in Town</i>	<i>Free Time</i>	
20:00-21:00					
21:00-22:00	<i>Dinner</i>	<i>Dinner</i>		<i>Dinner</i>	