

Advances in Atom and Single Molecule Machines
Series Editor: Christian Joachim

Philip Moriarty
Sebasti3n Gauthier *Editors*

Imaging and Manipulation of Adsorbates Using Dynamic Force Microscopy

Proceedings from the AtMol Conference Series,
Nottingham, UK, April 16–17, 2013

 Springer

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Philip Moriarty · Sebastián Gauthier
Editors

Imaging and Manipulation of Adsorbates Using Dynamic Force Microscopy

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Editors

Philip Moriarty
School of Physics and Astronomy
University of Nottingham
Nottingham
UK

Sebasti3n Gauthier
CMES-CNRS
Toulouse
France

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Foreword

There are many elegant examples of the manipulation of atoms and molecules on conducting and semiconducting surfaces using the scanning tunnelling microscope (STM), and a number of the chapters in this volume cite those studies. Dynamic force microscopy (DFM, also known as non-contact atomic force microscopy), however, opens up the possibility of constructing atomic-scale circuits, devices and machines on an *insulating* substrate. A key advantage of an electronically insulating surface supported by a robust bulk material is that the leakage current between interconnecting surface metallic contacts (i.e. ‘nano-pads’) will be very small, suppressing crosstalk between parts of the atomic-scale circuit. Similarly, in order to effectively electronically decouple the device from its environment, the electronic band structure of the bulk material must also be characterised by a large band gap.

These criteria impose important limitations on the choice of the supporting material, the surface preparation techniques (growth, cleavage, and thermal restructuring and/or reconstruction), the atomic-scale surface characterisation techniques used for analysis, and the final packaging of the circuit (using surface passivation, for example). A crude estimate of the surface tunnelling current intensity leads to the requirement of an electronic band gap larger than 6 eV in order to have surface leakage currents below a few picoamperes (at moderate operating voltages and for inter-contact distances of approximately 10 nm).

With these criteria in mind, and in parallel with the exploration of insulating supporting materials and surfaces, a number of important technological and scientific drivers can be listed. These span, for example, the development of single-molecule machines based on theoretical predictions and the generation of atomic-scale logic circuits at surfaces. The production of wafers comprising these types of devices is also important from an industrial point of view but requires exceptionally advanced processing and sensitive characterisation tools: the wafers must have close-to-perfect atomically ordered terraces. Currently, it is a major technological challenge to produce atomically flat terraces larger than 1 μm across without steps, emerging dislocations, or atomically scale defect. This type of atomically precise surface engineering paramount is important in order to scale-up surface circuit complexity.

The possibility of imaging the surface topography of such ideal surfaces with ‘subatomic’ scale resolution in real space is a prerequisite for the development of the single molecule and atomic logic gates whose development is pursued within the AtMol project. Traditional, optical, and electronic spectroscopies can still provide valuable information but simply do not have the necessary spatial resolution. Moreover, relatively high-energy electrons and/or photons can induce damage to the surface (and, indeed, of the bulk material below) induced by optical transitions or electronic charging effects. A key consequence has been the resurgence of the physicist’s interest in forces for imaging and manipulations at the atomic scale as presented in this, Volume 6 of the series.

Atomic force microscopy (AFM) has now been developed in many directions such as the contact, tapping and non-contact modes of operation, with a wide range of variations in terms of cantilever stiffness, oscillation frequency and amplitude. In the context of the atomic- and sub-molecular-scale manipulation necessary for the type of insulator-supported devices described above, NC-AFM seems now the instrument of choice. Pushed by the performance and the precision reached by the STM in the manipulation of single atoms and molecules and in the construction of atomic-scale circuits and molecular machineries, scientists developing NC-AFM instruments have an important benchmark in place to push force microscopy (and its associated spectroscopic capabilities) to the limits. They can provide the characterisation tools and manipulation protocols at the atomic scale that have been lacking for years at the surface of an insulator. Some research groups have also tried to push the STM to the frontier of the field emission regime, succeeding in imaging large electronic gap surfaces and single molecules on a metallic surface using tip-to-surface bias voltages of up to 10 V. This is very much at the limit of what an STM can do on insulating surfaces. Given that it is operating right at the limits of its capabilities, this application of the STM is not very practical for the atomic-scale operations required for structures and devices constructed or assembled at the surface of large bandgap materials.

The demonstrated ability to image an adsorbate on a large bandgap material is a superb scientific avenue not only in terms of acquiring detailed information on the electronic structure of a single atom or molecule but, moreover, to provide detailed access ‘inside’ the electronic cloud of the adsorbate (i.e. to image the atomic ‘architecture’ of a molecule). Even if the description of a molecule by its valence electronic density probability is a long-standing and well-illustrated feature of many textbooks, the recording of real-space experimental images of the ‘internal structure’ of an adsorbate is still a matter of considerable debate. Using a large electronic gap substrate is one way to minimise the direct electronic hybridisation between the atom, the molecule and its supporting surface. Strong hybridisation is very often encountered on metal and semiconductor surfaces. Here, the large number of atoms of the surface involved in strong electronic interactions with the adsorbate in essence act like a ‘quantum-to-classical’ convertor for the adsorbate. This coupling to the environment removes a key part of the quantum richness of the intrinsic electronic structure of, for example, a molecular adsorbate. In this context, measuring with ‘subatomic’ resolution the very local force between the end apex atom

of an AFM tip and the molecule's electronic cloud provides an entirely different method of accessing the internal electronic structure of the molecule as compared, for example, with field emission microscopy (FEM), transmission electron microscopy (TEM), or STM. The binding of single vertical molecule like CO to the apex of a scanning probe, as shown by Gross et al. at IBM Zurich, produces a fantastic force sensor to probe the interior of the electronic cloud of a molecule. This apex can also, in principle, be equipped with a high-spin atom for magnetic interrogation of the molecule's electronic structure opening up the possibility of intramolecular spin mapping.

The fundamental rationale behind those measurements lies in the problem of representing the very complex electronic structure of a many-electron molecule. Can the representation of such a complex electronic system be simply reduced to a pseudo-3D map of the ground electronic state of the molecule? Physisorbed at the surface of an oxide, a molecule is largely an isolated (but supported) minute piece of matter. At low temperature, its mechanical degrees of freedom will have some (or perhaps even total) classical behaviour due to quantum decoherence. This is a remarkable platform (or playground) for performing single-molecule mechanics, developing molecule motors and constructing molecular machines on a surface where the relation between the insulator characteristics and friction at the atomic scale remains to be explored. What role do the electronic degrees of freedom play in such a supported (or weakly coupled) situation? How can the corresponding many-body wave function be mapped (with local 'subatomic' resolution)? Is this local force spatial mapping closer in information content to the famous FEM images of a single isolated molecule (at the end of a tungsten tip) acquired by Muller in the mid-fifties, or to the direct space molecular orbital like images obtained by dI/dV constant current STM images? How might magnetism and the local mechanical response of a molecule be related? These are just a few questions posed by our new ability to probe the interior of the electronic cloud of a weakly adsorbed/interacting molecule.

A key additional advantage of an insulating surface is that it can be 'equipped' locally by nanoscale objects such as semiconductor nano-clusters, nanoscale metallic contacts ('nano-pads'), and even more functionalised nano-devices such as nano-gears. For example, ultraflat metallic nano-pads can be assembled directly on an insulating surface using a source of metal atoms or by transferring graphene nano-islands on the surface (with always the same constraint that these nano-islands must be defined with atomic-scale precision). Specific UHV growth and transfer printing techniques have now been developed for this purpose which preserve the atomic-scale order of the surface. NC-AFM can also play a key role in reconfiguring the surface location of adsorbed nano-objects.

One interesting phenomenon is the electronic interaction of an adsorbate with a single metallic nano-pad. The challenge here is the study of electron transfer and the consequent charging of a single atom or a single molecule at the atomic scale by a nearby metallic nano-island previously charged by simple electrostatic contact. To what extent, at the surface of an insulator, does this type of phenomenon occur? What is the lifetime of this charging effect and how does it depend on the large electronic band gap of the supporting material? Aside from these electrostatic and

electronic effects, mechanical interactions (such as the gearing between a molecule gear and a solid-state nano-gear) will also benefit from the use of an insulating surface to minimise the electronic friction encountered at the surface of, for example, a metal.

Following the investigation of the influence of an individual nanoscale object, the next logical step is the study of the interactions of atomic or molecular adsorbates with a number of nano-clusters. This will open up vast field of research for nano-electronic, nano-mechanics and, very soon, nano-magnetism and nano-optics (nano-plasmonics), which all will reach, in the years to come, atomic-scale precision. The adsorbate can be a single-molecule machine able to calculate, to 'memorise' data, or to perform mechanical work. By extension, it could also be an atomic-scale electronic circuit or complex mechanical machinery. In all these cases, avoiding through-surface inter-contact leakage current will remain a crucial objective.

The applied bias voltage required to drive nanoscale machinery or atomic-scale circuits via metallic nanoscale contacts will necessarily be smaller than the 6 eV band gap mentioned above. Having such a fully planar surface interconnection arrangement is the next frontier for the realisation of atomic-scale machines and technology. This is so crucial that this ongoing planarisation of atomic-scale technology is now triggering the development of a new class of instruments mixing near-field and far-field technologies and microscopies. These new microscopes, combining four low-temperature ultrahigh vacuum STMs or four NC-AFMs (or, indeed, a mix of both instruments) are now able to image and manipulate at the atomic scale in parallel and on the same surface. Such instruments incorporate an SEM, and sometimes a focused ion beam system, to ensure accurate navigation of the apices of four probes with respect to other nanoscale objects. With this new development, it is now the instrumentation which is adapted to the scale of the atomic machinery, rather than the use of 'scale-up' protocols (such as crystallisation) to enable the formation of a material compatible with the standard far-field characterisation and interconnection techniques.

These advances in instrumentation are underpinning the evolution of atomic-scale devices, machines and circuits towards a planar geometry. This planarisation in turn both opens a new window for experimentation and puts new challenges on the table including, in particular, the description of the observed phenomena using modern calculations tools. The combination of a large electronic gap surface, a bulk material as support, solid-state nanoscale structures for contacts and interconnects, and active single-molecule machines or atomic-scale circuit is a redoubtable challenge for quantum chemists. How can all these scales be encompassed, while also taking into account the precise electronic structure of each atom? Can it ever be only a semi-empirical description? What about the time-dependent responses of the atomic/molecular machinery? Can this be predicted from first principles before setting up the required instrumentation?

These exceptionally challenging questions have been largely outside the scope of the STM, for which metal and semiconductor surfaces were exploited for atomic-scale construction and for the development of the first elementary molecule

machines or atomic-scale circuits. The introduction of large bandgap surfaces, and the current availability of exceptionally high-precision non-contact AFM instrumentation, represent an exciting opportunity to experimentally realise single-molecule machines and atomic circuits previously only developed ‘in silico’.

To finish with, let me thank P. Moriarty and S. Gauthier for their time and patience in organizing the April 2013 AtMol workshop on non-contact atomic force microscopy-related techniques and all the participants of this workshop to have accepted to participate to this Volume 6.

Nottingham
April 2013

C. Joachim

Preface

This book, like others in the *Advances in Atom and Single Molecule Machines* series, stems from a two-day workshop associated with the Atomic Scale and Single Molecule Logic Gate Technologies (AtMol) project funded by the European Commission's Future and Emerging Technologies programme. AtMol, a four-year project, was launched on 1 January 2011, involves eleven research teams, and has as its central objective the design and fabrication of the first ever encapsulated single-molecule chip.

Scanning probe microscopy is at the very heart of the AtMol project, enabling the imaging and manipulation of matter at the atomic, molecular, and sub-molecular scales. As such, the workshop from which the chapters in this volume arise was funded both by AtMol and the ACRITAS Initial Training Network (www.acritas.eu), a Marie Curie Training Project also funded by the European Commission and which is focussed on the development of new techniques and methods in atomic force microscopy.

The workshop in question, *Imaging and Manipulating of Adsorbates Using Dynamic Force Microscopy*, was held at the University of Nottingham during 16–17 April 2013. The contributions included in this volume represent a 'snapshot' of the state of the art in dynamic force microscopy (DFM, also called non-contact atomic force microscopy) at that time and cover a variety of fascinating topics including the accurate extraction of tip–sample forces from measured frequency shift curves; the imaging and manipulation of single atoms, molecules, clusters, and dangling bonds; the role of the Pauli exclusion principle in high-resolution DFM; and the combined mechanical and electrical properties of individual molecules.

At the time of writing, DFM is at an intriguing juncture in the evolution of the capabilities of the technique. There has been significant excitement about the possibility of imaging intramolecular, and, in particular, inter-molecular bonds, over the last 18 months or so. It has now become clear that the latter, i.e. the observation of contrast maxima *between* molecules in DFM images, has to be interpreted very carefully indeed. As with any scanning probe technique, the geometric and electronic structure of the apex of the tip (and its associated chemical functionality) is just as important in the imaging mechanism as the sample. This

convolution can be particularly severe in the so-called Pauli exclusion regime of imaging which was pioneered by IBM Zurich (Gross et al.) in 2009 (and which is increasingly becoming the norm for the acquisition of ultrahigh resolution DFM images).

As one of us (PM) and co-authors discuss in the chapter “[Pauli’s Principle in Probe Microscopy](#)” of this volume, the contribution of the dynamics and mechanics of the tip apex plays an exceptionally important role in generating image contrast. Seeing is not necessarily believing with any imaging technique, and this is especially true of scanning probe microscopy. On the other hand, there remains immense potential for the use of a range of different functional probes (including, but also moving beyond, CO, which is used extensively for intra molecular imaging at present) in DFM, enabling analysis of a variety of physicochemical phenomena. These include molecular magnetism, as also mentioned in the Foreword to this book. The exciting challenges and opportunities for ultrahigh resolution DFM will be discussed and debated in a workshop in Prague in February 2015 which has been organised by Pavel Jelinek, author of chapter “[Theoretical Challenges of Simultaneous Nc-AFM/STM Experiments](#)” of this volume (see below).

In the chapter “[Mechanical and Electrical Properties of Single Molecules](#)”, Thilo Glatzel provides a comprehensive overview of a number of the considerable advances of the Nanolino group at the University of Basel in imaging and characterising the mechanical and electrical properties of single molecules. For all of the reasons outlined by Christian Joachim in his Foreword, there are fundamental and technologically important motivations for the use of insulating, as opposed to metal or semiconductor, substrates as a ‘platform’ for molecular adsorption. Glatzel’s overview gives a good indication of the state of the art in the field and also highlights key differences between the properties of molecular adsorbates on metallic and insulating substrates.

Sugimoto and colleagues at Osaka University have been responsible for many of the key advances in atomic manipulation and single atom control using DFM. Prof. Sugimoto’s chapter reviews some of the work of the Osaka group (and their collaborators) in developing a number of fascinating and high-precision protocols for the controlled positioning of single atoms, with a particular focus on the lateral translation of silicon adatoms. Sugimoto discusses how the tip apex in a DFM manipulation experiment can be characterised through measurement of the short-range chemical force and, in particular, by using the maximum attractive force as a ‘metric’ or a diagnostic. In addition, however, he stresses how tip geometry—*asymmetry in particular*—plays a central role in determining the probability for manipulation events to occur.

In a second contribution from the Nottingham group,¹ Andrew Stannard and Adam Sweetman explore the difficulties and subtleties associated with extracting accurate quantitative force measurements from dynamic force microscopy measurements of frequency shift versus tip–sample separation. Although DFM is an

¹Disclaimer: one of the editors (PM) is a member of this group.

exceptionally powerful tool for the measurement of tip–sample force fields and potential energy landscapes, it is far from trivial to extract accurate and reliable quantitative force values from the primary experimental observable, i.e. the frequency shift (Δf). Subtraction of the contribution of the long-range van der Waals interaction, in which the short-range chemical force curve is ‘buried’, is a perennial, and particularly thorny, issue. Stannard and Sweetman describe protocols for the systematic treatment of $\Delta f(z)$ curves (where z represents the tip–sample separation) so as to minimise the uncertainties in converting the experimental data to a plot of $F_{\text{SR}}(z)$, i.e. the short-range force curve associated with the interaction of just the atom/molecule terminating the tip apex with the underlying sample surface atom(s).

The chapter “[Theoretical Challenges of Simultaneous Nc-AFM/STM Experiments](#)”, authored by Pavel Jelinek of the Academy of Sciences of the Czech Republic, is an authoritative and fascinating review of the current state of the art in theoretical descriptions of ‘hybrid’ scanning tunnelling microscopy (STM)—DFM measurements. Jelinek’s group has carried out pioneering and influential work on this topic, and he provides an accessible and readable introduction—perhaps written with experimentalists in mind—of the latest developments in the use of density functional theory, coupled with a Green’s function² approach, to simulate not only the geometric and chemical interactions occurring at the tip–sample junction, but to accurately predict the (far from equilibrium) tunnel current driven through the system by the application of a bias voltage. The question of just how the distance dependence of the tunnel current compares to that of the short-range chemical force has been a long-standing issue in scanning probe microscopy, and Jelinek discusses the key theoretical advances that have elucidated the underlying physics. He also highlights the fascinating, and ‘far beyond perturbative’, influence of the formation of a covalent bond on the tunnelling barrier experienced by electrons flowing from tip to sample (or vice versa).

The next chapter, written by Clemens Barth (CNRS, Aix-Marseille University), explores the use of DFM to manipulate objects rather larger than the single atom/molecule adsorbates discussed thus far: nanoscale clusters. As discussed in the Foreword, nanoscale clusters and nanoparticles have a key role to play in enabling the development of next-generation atomic circuitry, particularly with regard to interfacing single atom and sub-molecular functionality to the microscopic, and ultimately macroscopic, world. Barth describes the challenges underpinning controlled translation of clusters and discusses how his group has developed techniques to control the positioning and dynamics of Au nanoparticles on NaCl substrates. The importance of the wide electronic band gap of insulating surfaces and substrates was also stressed repeatedly by Joachim in the Foreword, and it is encouraging that Barth shows that not only is nanoparticle manipulation on wide bandgap substrates achievable, but that the presence of surface defects does not

²Given the venue for the workshop from which this volume stemmed, it would be remiss of me not to highlight that George Green, of Green’s function fame, did his mathematics while working as a miller in Nottingham in the nineteenth century.

preclude controlled positioning. Indeed, the chapter “[Manipulation of Metal Nanoparticles on Insulating Surfaces](#)” provides compelling evidence that defects are an integral part of the manipulation process, first stabilizing, and then acting in concert with the nanocluster as it is moved across the surface by the DFM tip.

In the chapter “[Imaging of Defects on Ge\(001\):H by Non-contact Atomic Force Microscopy](#)”, we remain with the theme of defect-mediated interactions but return to the imaging and quantitative analysis of semiconductor, rather than insulator, surfaces. Bartosz Such (Jagiellonian University, Kraków) focuses on a prototypical passivated, i.e. low free energy, semiconductor surface—hydrogen-terminated Ge (100)—and describes the significant differences between force curves acquired over passivated surface regions as compared to those measured above single dangling bond defects (i.e. regions of the surface where a Ge atom is not hydrogen ‘capped’). As has also been observed for the H:Si(100) surface, the chemically inert hydrogen-passivated regions are associated with a negligible attractive interaction with the DFM tip. As such, atomic resolution imaging is achieved within the range of the tip–sample interaction potential where the repulsive component of the total force plays a significant role (as discussed in the chapter “[Pauli’s Principle in Probe Microscopy](#)” in relation to the Pauli exclusion principle). Above a dangling bond defect, however, there is a much stronger attractive force due to the short-range tip–sample interaction arising from the formation of a chemical (presumably covalent) bond. Such discusses how the force of this single dangling bond can be measured.

We subsequently return to a discussion of insulating surfaces in the chapter “[Adsorption Structures of Amino Acids on Calcite\(104\)](#)” but here the focus is on calcite rather than the alkali halides exploited by Barth et al. for the nanocluster manipulation described in the chapter “[Manipulation of Metal Nanoparticles on Insulating Surfaces](#)”. As Felix Kling, Markus Kittelmann and Angelika Kühnle discuss, calcite is a fascinating and exceptionally important substrate in the context of the study of biomineralisation. They exploit the cleavage plane of calcite, i.e. calcite(104), as a platform and template for the self-assembly of five different amino acids. Although the larger molecules of those they studied, namely tryptophan, tyrosine, and aspartic acid, exhibit strikingly similar behaviour on the calcite surface with regard to the superstructures they adopt, the smaller amino acids (glycine and alanine) behave in a very different manner. A rather elegant aspect of Kling and co-worker’s study is that they unambiguously define molecular chirality from a careful analysis of the relationship of the alignment of adsorbed superstructure with the crystallographic directions of the underlying substrate.

The final chapter of this volume, by Antoine Hinaut and colleagues, continues with the topic of molecular adsorption on an insulating surface but has a specific focus on the electrostatic properties of the adsorbed molecules (which, like the amino acids studied by Kling et al., form highly ordered superstructures on the substrate). Hinaut et al. have carried out a combined DFM and Kelvin probe force microscopy (KPFM) study of a triphenylene derivative, 2,3,6,7,10,11-hexacyano-propyl-oxytriphenylene, on a KBr surface. A systematic, comparative, and detailed study of the KPFM data acquired above the bare KBr surface and on the molecular islands showed that the Kelvin probe signal, which provides a measure of the local

work function of the sample, could be interpreted in terms of the conformation-dependent polarisation of the molecular overlayer. Classical electrostatic calculations of the KPFM signal, based on a spherical tip apex, were found to provide good agreement with the experimental data. Given that there has been considerable discussion and debate regarding the origin and physicochemical underpinnings of KPFM measurements, Hinaut et al.'s work provides key insights into the extent to which intuition and models from classical physics can be used to interpret Kelvin probe data.

Taken together, the nine chapters in this volume capture the state of the art in dynamic force microscopy at an intriguing and exciting time in the evolution of the field. Five years on from the pioneering work of Leo Gross and colleagues at IBM Zurich, who showed that the 'architecture' of adsorbed molecules could be resolved in exquisite detail, there remain a variety of exciting questions to be addressed about the ultimate limits of DFM. Christian Joachim has touched on some of these open questions in his Foreword, and we echo his comments regarding the possibility of measuring local spin density and pushing the magnetic measurement capabilities of the instrument, as explored by Schwarz, Wiesendanger and colleagues at Hamburg, to wider, more challenging, horizons. The recent availability of commercial instruments capable of carrying out DFM in relatively high magnetic fields will of course provide an impetus for this direction of research.

Developments in instrumentation will clearly proceed apace—Franz Giessibl, whose farsighted introduction of the qPlus sensor (followed by the commercialisation of this technology by companies such as Omicron Nanotechnology (now part of Oxford Instruments) and Createc) has driven the wide adoption of DFM in labs across the world, continues to innovate with regard to both sensor design and the application of the qPlus technique to exciting scientific problems. As we write this in early 2015, DFM remains a very slow technique—the effective image generation bandwidth is sub-Hz rather than kHz or MHz. There thus remains particularly exciting scope for the development of DFM instruments capable of providing much greater temporal resolution, to complement the impressively high level of spatial resolution that is now possible with DFM.

We thank the European Commission's ICT-FET and Marie Curie programmes for their financial support in organizing the joint ATMol-ACRITAS workshop and the staff of Springer Verlag (particularly Judith Hinterberg) for their help in producing this book. We are also very grateful to Christian Joachim for leading the AtMol project and for his advice and patience throughout the preparation of this book. Finally, we would like to thank all of the authors who have contributed their work to this volume.

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Toulouse
January 2015

Philip Moriarty
Sebasti n Gauthier

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