Modeling Single-Molecule Junctions: Novel Spectroscopies and Control

Summary

The workshop "Modeling Single-Molecule Junctions: Novel Spectroscopies and Control" ran in the Seminaris Campus Hotel in Berlin from the 14th to the 16th of October, 2013. The objective of the workshop was to develop a theoretical roadmap toward the quantitative modeling of novel spectroscopies and control scenarios in single-molecule junctions. For this, the meeting brought together and promoted interactions between researchers in surface science, molecular electronics, single-molecule pulling and control theory. While the focus of the meeting was on theoretical developments, the group of invited speakers consisted of leading theoreticians and experimentalists who are actively working on different aspects of the problem.

Figure 1 Organizers and participants – Modeling Single Molecule Junctions: Novel Spectroscopies and Control, Berlin 2013.

The ESF funding provided for the meeting was supplemented with funds by the grants of two of the organizers. The Max Planck Society provided logistic support in the organization and the conference materials. The meeting was promoted in the Psi-K and MD News email lists, and through the invited speakers. We had a diverse group of 62 participants with 23 invited speakers, 4 contributed talks from early-career researchers and 35 contributed posters. The workshop participants came from 12 different EU countries, Switzerland, USA, China and Israel. The group photo is shown in Figure 1. The conference consisted of 3 full days of activities, including 2 poster sessions and 2 social events. Invited talks were limited to 30 minutes with 10 minutes reserved after each talk for discussion. Between sessions, ample time was reserved to facilitate informal discussions among participants.

The talks were of a very high standard and covered three key areas: 1.Multiscale modeling of molecule-surface and molecule-probe interactions. 2. Theoretical description of molecular imaging and transport across single molecules. 3. Light, voltage and force-driven phenomena in single-molecule junctions. The discussion was very active throughout the meeting, both during the formal sessions and in the coffee/meal breaks and poster sessions. The speakers were asked to comment directly on a number of prescribed questions and we have compiled a summary of the collective vision for the field that emerged from this discussion. In addition, the meeting resulted in several new collaborations among the participants.

We enjoyed the meeting immensely and have received very positive feedback from a number of participants. It is expected that it will have significant impact on the development of this topic in Europe and beyond.

Generalities and Objectives

Detailed modeling is needed to understand and develop single-molecule junction measurements. However, theoretical modeling of nanojunctions is extraordinarily challenging because of their multiscale nature in both time and space. The problem is multiscale in space because it deals with the properties of a molecular system on a nanometer scale that interacts with, and is strongly influenced by, a macroscopic surface. In time, because experimentally relevant molecular motions can span timescales that range from vibrations on a femtosecond timescale to rare molecular events with timescale longer than a microsecond. The presence of external stimuli further complicates the modeling, by driving the system away from structural and electronic equilibrium.

The objective of the meeting was to bring together researchers from a range of fields related to single molecule junctions and to use this forum to highlight both the state-of-the-art for the field and to engage in a comprehensive discussion of the challenges for the future. The 23 invited speakers and 4 contributed presentations were chosen to focus the meeting on three key areas for the field: 1. Multiscale modeling of molecule-surface and molecule-probe interactions; 2. Theoretical description of molecular imaging and transport across single molecules; 3. Light, voltage and force-driven phenomena in single-molecule junctions.

Our invited speakers were both theorists and experimentalists (17 and 6 respectively). We had had an extremely positive response to our invitations for invited speakers, and this was reflected in the very high standard of the talks at the meeting. We had a mix of speakers with both researchers with a long history of working on molecular junctions and researchers whose areas of expertise, while critical for understanding junctions, are not represented at a standard “molecular electronics” meeting. In particular, our inclusion of molecule-surface interactions, multiscale methods, plasmonics and theoretical methods developed for understanding biological systems, made this workshop an interesting melting pot of new ideas. The full program for the meeting, included in the appendix, gives a more detailed picture of the talks we had (including titles).

We also had two very active poster sessions during the meeting with 35 posters presented. The time during the poster sessions, as well as coffee breaks, lunches and dinners, was well used for active scientific discussion amongst the participants.

Scientific Content of the meeting

1. The complexity of molecules on surfaces

Our workshop featured 7 talks (2 experimental and 5 theoretical) on challenges towards a better understanding of molecules on surfaces in theory and practice. The workshop started with an inspiring talk by S. Tautz (Juelich) on their recent landmark experiments on using sensitive atomic force microscopy to measure the adsorption potential on large molecules on metal surfaces. This talk provoked quite some discussion on both the interpretation and accurate modeling of these experiments. The following talk was given by N. Moll who discussed recent experiments and calculations at IBM-Zuerich on "seeing" the electronic structure and adsorption geometries of single molecules on surfaces. The talks by M. Rohlfing and W. Liu nicely complemented the two experimental talks. In fact, both of them referred to and compared their calculations to experiments carried out in Juelich and IBM-Zuerich. All these talks clearly highlighted the necessity of accurately modeling van der Waals interactions for obtaining reliable structures and stabilities of molecules on surfaces.

The talk by L. Kronik highlighted yet another problem with traditional density-functional theory (DFT): the so-called self-interaction error. This error leads to many artifacts in DFT calculations, in particular it leads to lousy electronic properties. Kronik has presented several ways to correct the self-interaction error in an efficient manner.

The two talks by J. Behler and G. Csanyi discussed recent developments in using machine learning techniques (neural networks and gaussian potentials) for extending the time and length scales of first-principles simulations. Behler presented significant achievements that included full-scale neural-network simulations of realistic surface models with thousands of atoms. The limitation is that his models can only be used for systems containing only up to a few chemical elements. Csanyi gave an insightful presentation on the theory and art of constructing approximate potentials from first-principles binding energy data. He highlighted a few challenges that have to be solved in the construction of atomistic models towards the goal of accurately studying the dynamics of complex systems.

2. Charge and heat transport through single molecules

Charge transport in molecular junctions has underpinned much of the development in this area over the last fifteen years. In more recent years, researchers have increasingly branched out to measure light-induced dynamics and force in these junctions (included in separate sections below) but also to heat transport and thermoelectric properties of the junctions. These topics were addressed in 6 experimental talks, 7 invited theoretical talks and 3 contributed theoretical talks.

The contributions from experimentalists (Wandlowski, Venkataraman, Grill, Pascual, Hihath, Scheer), highlighted the challenges in reproducibly contacting molecules in junctions and reliably determining molecular conductance. Statistical approaches (Wandlowski, Venkataraman, Pascual, Hihath), where the junction is repeatedly formed and broken allow for reliable measurements but pose a challenge for theory as the junction structure is unknown. More controlled single junction measurements (Grill, Scheer) provide a very detailed picture of the junction in question for theoretical modeling, but may involve an investigation of a “special” system.

The contributions from theory took a number of different directions. There was a diverse range of chemical systems studied from small molecules on surfaces (Paulsson), to cross-conjugated systems (Lykkebo), systems with unpaired spins (Herrmann, Bagrets), saturated systems (Mirjani), carbon/graphene based materials (Cuniberti, Evers) and biological/biologically inspired systems (Beratan, Elstner). Such a range of systems, necessitated different theoretical treatments and raised different challenges for the area. For example, the systems with unpaired spins introduced the possibility of Kondo physics and the biological systems raised questions about the charge transport mechanism, both of these have very specific consequences for the nature of the calculations that need to be performed and these were outlined by the speakers. There was also a discussion of how higher level theoretical methods could be used to go beyond the standard tools used for calculating charge transport (Galperin).

The relationship between charge and heat in molecular junctions was also discussed by a number of researchers. Current induced heating (Pecchia, Paulsson, Lykkebo, Cuniberti) and its associated spectroscopic marker, inelastic electron tunneling spectroscopy (experimental: Hihath, theoretical: Paulsson, Lykkebo) were discussed, as well as

thermoelectric response (experimental: Venkataraman, theoretical: Cuniberti) and heat transport (Cuniberti).

3. Light and voltage-induced dynamics in junctions

Another important development in single-molecule junctions that was represented in this meeting is the use of light and voltages to induce dynamical events. Rubio described general DFT-based methodology that can be used to capture the light-induced time evolution of electronic systems. Masiello described how to model plasmons in nanoparticles induced by light or by electron scattering. May described the modeling of time-dependent transport in junctions using master equations, including a description of the effect plasmons on the dynamics. Hihath described an experimental approach that can be used to resolve ultrafast events in junctions via current measurements. Scheer described experiments of light-induced transport switching in photochromic molecules.

4. Force spectroscopy in molecular junctions

A point of focus in this meeting was the use of force spectroscopy in the context of single-molecule junctions. Since this is currently a hot topic in this area, several of the experimentalists in the meeting discussed this point from different angles. Specifically, Tautz, Grill, Moll and Pascual described ultra high vacuum experiments, while Venkataraman described room temperature measurements. Tautz described pioneer experiments demonstrating how force and conductance measurements can be used to directly measure adsorption energies and molecule-surface van der Waals potentials. Venkataraman described experiments that show that even room temperature force-extension measurements can be used to quantify van der Waals interactions at metal/organic interfaces, and how the force probe can be used to tune the molecular conductance by altering the conformation of the junction. Moll described the IBM efforts to image molecules on surfaces with atomic resolution using functionalized AFMs, and how these images could be understood using electronic structure methods. Grill showed experiments measuring the conductance of rigid and flexible single molecules as a function of elongation. Makarov complemented this picture by introducing the theory of single-molecule pulling including an enlightening description of the how forces can be used to modify chemical reactivity. In the contributed presentations, Franco and Solomon described theoretical efforts to model the transport properties of single molecules as they are mechanically elongated.

Discussions during the meeting

While we had speakers from a range of areas, we wanted to maintain a central focus for the discussion. To this end, we asked all speakers to include one slide in their presentations where they comment on the following points :

- What is the biggest challenge in developing an effective model for nanoscale junctions that is both fast and accurate? Are there good approximations we can make?
- What theoretically relevant information should we extract from single-molecule experiments? If not measured directly, how do we do that?
- What kind of novel control schemes can we develop at the single-molecule junction level?
- How can theory help experimental progress in this area, and vice versa?

We found this to be an incredibly effective device for stimulating discussion at the meeting and received large number of interesting suggestions. Some of the suggestions fell neatly along the lines we had anticipated with our choice of speakers and topics for

the meeting (for example with regard to the electronic structure methods required to model these junctions), while others were very different. Throughout the meeting we noted the suggestions made and compiled a summary that was presented to the meeting in our closing remarks. This summary is illustrated in Figure 2.

Under the broad area of the challenges facing molecular junctions, there were six sub-areas. The most overarching is "The strategy" and here the discussion was focused on the approach to the problem in the broadest sense. Within this area, "What's next?" dealt with the question of how the field should progress. "Do we need a black box?" and "Transport mechanism" were concerned with the strategy that theoretical researchers should take in their method development and "Feedback between theory and experiment" was a discussion on how we could effectively work together for optimal progress.

The discussion surrounding "The observables" focused on both the traditional information that can be extracted from experiments and that which is coming from emerging techniques. This topic area drew on the full range of invited speakers we had present and highlighted the interrelationships between various observables.

"Statistics" was a discussion area that arose out of the nature of the experimental techniques (where observables are determined statistically over many measurements) and how theory should respond to this complexity. The discussion highlighted that there is useful analysis to be performed with both the statistically averaged data and the results from single measurements but in both cases theory needs to embrace the complexity of this problem rather than simply considering idealized situations.

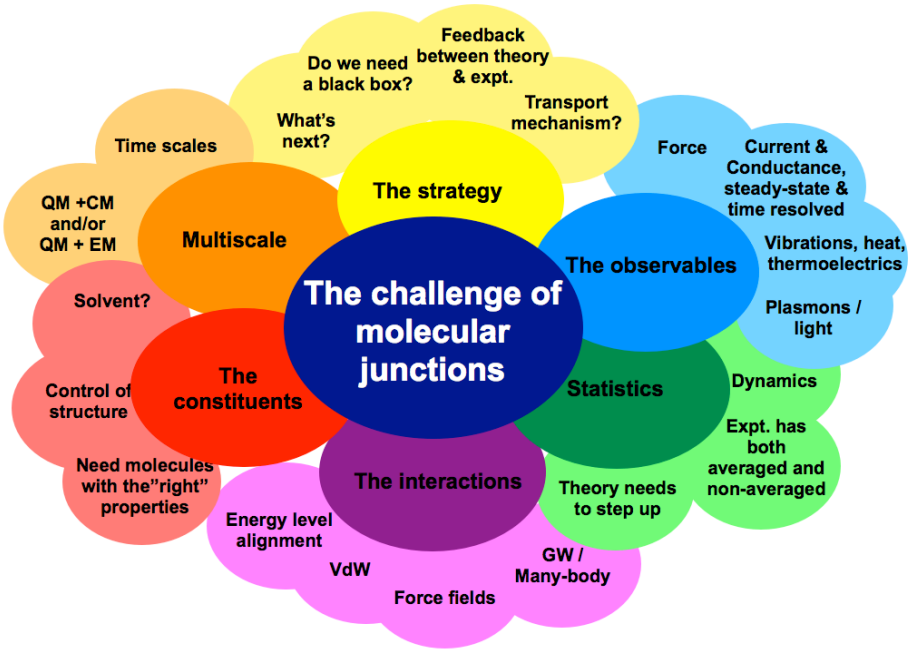


Figure 2 The challenges highlighted by our speakers in their talks and the discussion throughout the meeting.

“The interactions” highlighted the challenges for theoretical methods in dealing with nano-scale systems that fall outside the traditional domains of chemistry and physics. The most sophisticated chemical methods are not usually capable of dealing with large metallic electrodes and the most sophisticated methods from physics do not always offer the best descriptions of molecular electronic structure – this challenge emerges both in the problems of “energy level alignment”, the inclusion of Van der Waals forces (“VdW”) and “many-body/ GW”. In order to capture the dynamics that are present in the experiments and in an effort to move to statistically significant numbers of calculations, there is also a challenge in developing “force fields” to attack this problem.

Finally, “multiscale” was a challenge area that emerged from the theoretical talks as problems associated with the huge range in “time scales” and length scales emerged. The discussion focused on how to embrace this challenge by combining quantum mechanical methods with more approximate schemes to model the systems involved.

Assessment of the Results

The enthusiastic response we had from both invited speakers and other registered participants reflected the demand that exists in the community for these kinds of workshops. We have received feedback from a number of participants indicating that the program was very effective for presenting a range of exciting new developments in the field, stimulating their thinking and giving good time for discussions.

Compared with other “molecular electronics” meetings, we believe there are two areas that set this meeting apart. Firstly, we had a very structured program that allowed us to have a clear topic area (single molecule junctions) while at the same time bringing in researchers from related disciplines without losing focus. This has a two-fold benefit in that it not only broadens the outlook of researchers who consider themselves to be working on molecular electronics but also highlights to researchers in related disciplines how they can help and profit from this field. As an example, Behler spoke about developing neural network potentials for atomistic simulations and comment on the fact that previously he had always strived for the most universal scheme (i.e. an approach that could be applied to any problem involving a certain subset of elements). The problem for this approach is that it becomes very difficult to include a large number of elements. However, if he considered how to develop these potentials for molecular junctions, the chemical nature of the system means that certain simplifications can be made and a different strategy could be adopted. This sort of cross-pollination between fields is extremely useful and emerged naturally from our meeting.

The second area in which this meeting was particularly special was the high quality of discussion. This encompassed both the details of the scientific talks but also our general challenge areas. The “roadmap” of challenges that emerged from the meeting is an extremely useful tool to have as we move forward and a fantastic record of the status of the field today. We can thoroughly recommend the use of “homework questions” to invited speakers before a meeting as a device to stimulate focused discussion and will certainly use them ourselves in the future.

Over the next 1-2 years, we will follow the developments in the field and determine if and when a follow-up workshop is required. The record we have from the discussion at this meeting provides a great starting point for future workshops to assess how the area has progressed and which areas are lacking. Anecdotally, we know that this workshop allowed many researchers to strengthen existing international collaborations, as well as

developing new collaborations. While such output is hard to quantify, we feel that the environment we created with meals together and good time for discussion outside the sessions, played a significant part in fostering this interaction.

Feedback from some of the participants

It is also relevant to note how was the experience of other participants. To this end here we include some of the comments that were sent to us via email as a follow up to the meeting.

Leeor Kronik

For me, this was an excellent meeting! Several things stood out in particular: First, it had a well-defined focus but wasn't too narrow. Second, it had just the right balance between theory and application. Third, it left ample time for in-depth discussions. Thank you again for putting this together and for the kind invitation!

Ferdinand Evers

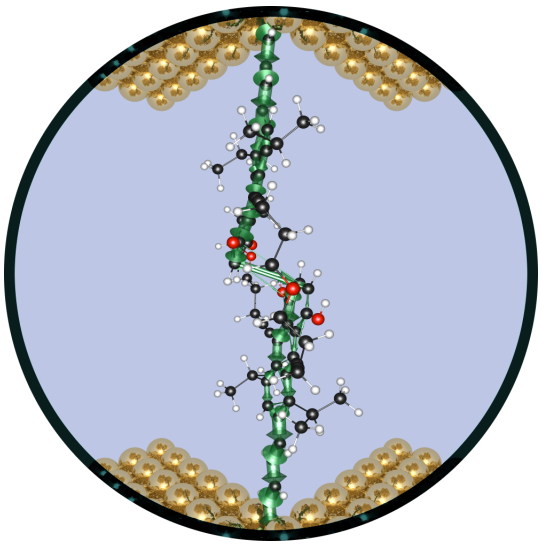
1. It was wonderfully organized and therefore very stimulating with respect to communication between scientists. (location, dinner). What I remember most vividly from the meeting are the conversations that took place at various occations (coffee break, dinner, poster session...) I have had the opportunity to deepen several existing national and international collaborations and formulate new project, to meet new cooperation partners (two very good postdoc candidates !) and to talk about very important community related topics, like the future organization of conference series or general funding issues.
2. Top speakers have been invited to share their results with a broader community from made up from people of neighboring fields, such as surface sciences. The level of all contributions was very high and the discussions most useful.
3. The FU Berlin (together with the FHI) underlined once more its status as a center of excellence in ab-initio / surface physics / chemistry related research.
4. The program was special in the sense that it brought together people that work on related subjects but that do not belong to exactly the same inner communities and for that reason don't meet, usually. An example was the field of nano-plasmonics, that seems to develop significant overlap with Molecular Electronics very quickly. This is very encouraging to see.

With my best wishes and a good deal of gratitude!

Gianaurelio Cuniberti

Thanks for the great workshop. It had an ideal format and plenty of informal discussion chances. I really enjoyed it.

Appendix



Modeling Single-Molecule Junctions: Novel Spectroscopies and Control

October 14th - 16th, 2013

Seminaris Campus Hotel
Berlin, Germany

Organizers

Ignacio Franco (University of Rochester)
Gemma Solomon (University of Copenhagen)
Alexandre Tkatchenko (Fritz Haber Institute)

http://www.fhi-berlin.mpg.de/th/msmj2013

1. General information

Scope

Emerging technologies that allow the application of light, forces and voltages on single-molecule junctions have the potential to provide a powerful avenue for molecular control and to yield novel highly discriminating multidimensional spectroscopies. The challenge for theoretical studies is to correctly capture the complexity of these multi-scale, non-equilibrium systems. This workshop seeks to provide a roadmap to navigate the theoretical challenges by bringing together and fostering interactions between researchers in surface science, molecular electronics, single-molecule pulling and control theory.

Key Topics

I. Multiscale modeling of molecule -surface and molecule- probe interactions

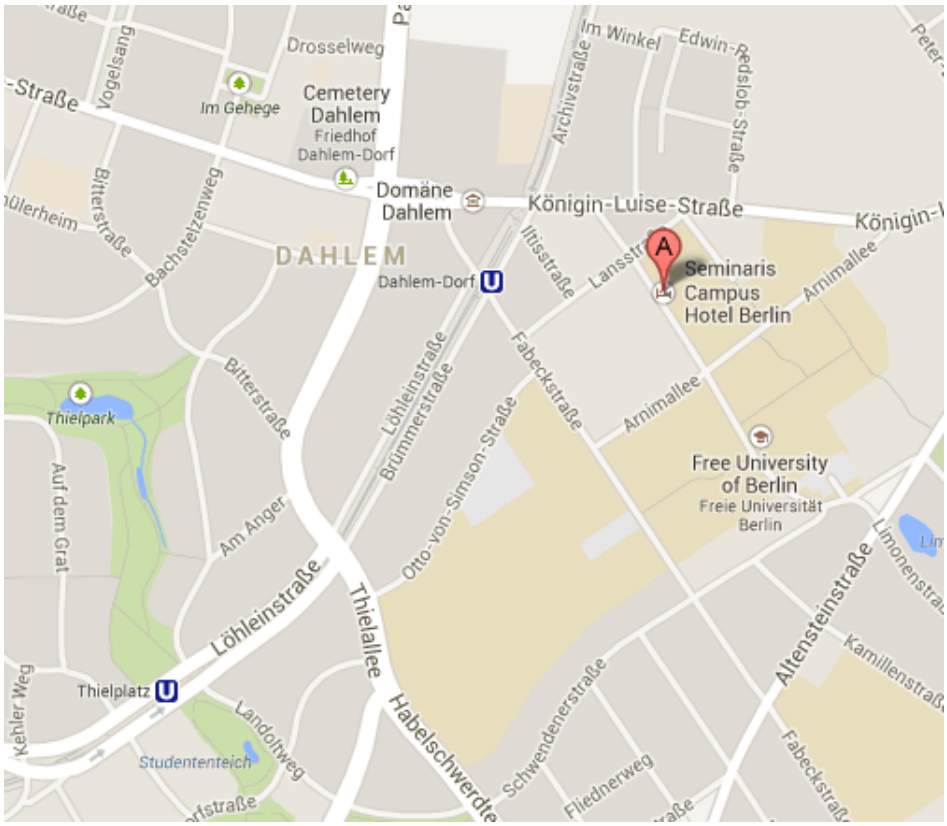
II. Theoretical description of molecular imaging and transport across single molecules

III. Light, voltage and force-driven phenomena in single-molecule junctions

2. Location & Map

Seminaris Campus Hotel, Takustrasse 39, 14195 Berlin, Tel. +49 30 557 7970 (from outside Germany); 030 557 7970 (from Germany)

Closest train station: Dahlem-Dorf (U3)



3. Program

Invited talks are 30 minutes long followed by 10 minutes of discussion. Contributed talks are 15 minutes long followed by 5 minutes of discussion.

Monday, October 14, 2013

08:00 – 08:50 **Registration**
08:50 – 09:00 **Welcome**
09:00 – 12:30 **The complexity of molecules on surfaces**

09:00 – 09:40 **Stefan Tautz** (Forschungszentrum Jülich)
"Precise adsorption energies and molecule-surface van der Waals potentials from force measurements"
09:40 – 10:20 **Nikolaj Moll** (IBM Research - Zurich)
"Imaging Atoms and Bonds by Atomic Force Microscopy"
10:20 – 10:50 Coffee Break
10:50 – 11:30 **Michael Rohlfing** (University of Muenster)
"Structure and spectra of organic molecules on silver from first principles"
11:30 – 12:10 **Leeor Kronik** (Weizmann Institute of Science)
"The derivative discontinuity: origins, hiding places, and implications for transport"
12:10 – 12:30 **Wei Liu** (Fritz Haber Institute of the Max Planck Society)
"Reliable Modeling of Complex Organic/Metal Interfaces"

12:30 – 13:50 **Lunch**

13:50 – 15:50 **Novel spectroscopies in junctions I: conductance, forces and beyond**

13:50 – 14:30 **Thomas Wandlowski** (University of Bern)
"Charge Transport with Single Molecules: An (Electro-) Chemical Approach"
14:30 – 15:10 **Ferdinand Evers** (Karlsruhe Institute of Technology)
"Quantum size effects in the response properties of single molecules"
15:10 – 15:50 **Latha Venkataraman** (Columbia University)
"Mechanics of Single-Molecule Junctions"

15:50 – 16:20 Coffee Break

16:20 – 17:40 **Multiscale Modeling**

16:20 – 17:00 **Joerg Behler** (Ruhr-Universität Bochum)
"Extending the Length and Time Scales of Atomistic Simulations Using Neural Network Potentials"
17:00 – 17:40 **Gabor Csanyi** (University of Cambridge)
"Theory and practice of creating first principles-based interatomic potentials"

17:40 – 18:40 **Poster Session I**

From 19:00 **Chinese Style Dinner:** China City, Leipziger Str. 46, 10117 Berlin-Mitte /

closest train station U2 Spittelmarkt http://www.china-city.eu/

Tuesday, October 15, 2013

09:00 – 12:10 **Novel spectroscopies in junctions II: light and voltage-induce dynamics**

09:00 – 09:40 **David Masiello** (University of Washington)
"Optical-and electron-driven plasmonic environments and their affect upon nearby resonant molecular media"
09:40 – 10:20 **Angel Rubio** (University of the Basque Country)
"Light-induced dynamical processes in finite and extended systems from TDDFT"
10:20 – 10:50 Coffee Break
10:50 – 11:30 **Elke Scheer** (University of Konstanz)
"Transport properties of optically driven molecular switches"
11:30 – 12:10 **Volkhard May** (Humboldt-University, Berlin)
"External Field Control of Sequential Charge Transmission through a Molecular Junction"

12:10 – 12:20 Group picture

12:20 – 14:00 **Lunch**

14:00 – 15:30 **Poster Session II**

15:30 – 18:30 **Novel spectroscopies in junctions III: conductance, forces and beyond**

15:30 – 16:10 **Michael Galperin** (University of California San Diego)
"Charge and energy transport in molecular junctions"
16:10 – 16:50 **Dmitrii E Makarov** (University of Texas at Austin)
"Mechanically driven quantum transitions: Quantum Zhurkov-Bell Formula"
16:50 – 17:10 Coffee Break
17:10 – 17:50 **Leonhard Grill** (University of Graz)
"Voltage-dependent charge transport through single molecular wires"
17:50 – 18:30 **José Ignacio Pascual** (CIC nanoGune)
"Forces and photons from molecular junctions"

From 19:00 **Berlin Style Dinner:** Brauhaus Lemke, Hackescher Markt, Dircksenstr. 143,

S-Bahnbogen, 10178 Berlin-Mitte
Closest train station U2 Klosterstrasse from there app. 5 min. walk
http://www.brauhaus-lemke.com

Wednesday, October 16, 2013

09:00 – 10:20 **Simulation of charge transfer in complex environments**

09:00 – 09:40 **David Beratan** (Duke University)
"Transport through Soft, Wet, Fluctuating Biomacromolecules"
09:40 – 10:20 **Marcus Elstner** (Karlsruhe Institute of Technology)
"Simulation of charge transfer in complex systems"

10:20 – 10:50 Coffee Break

10:50 – 12:10 **Novel spectroscopies in junctions IV: conductance, forces and beyond**

10:50 – 11:30 **Joshua Hihath** (University of California, Davis)
"Electromechanical Properties of Atomic and Molecular Junctions"
11:30 – 11:50 **Carmen Herrmann** (University of Hamburg)
"Electronic communication through molecular bridges"
11:50 – 12:10 **Fatemeh Mirjani** (Delft University of Technology)
"Charge transport across insulating self-assembled monolayers"

12:10 – 13:40 **Lunch**

13:40 – 16:50 **Novel spectroscopies in junctions V: inelastic transport, thermoelectrics and Kondo effect**

13:40 – 14:20 **Gianaurelio Cuniberti** (TU Dresden)
"A bottom-up route to enhance thermoelectric figures of merit in graphene nanoribbons"
14:20 – 14:40 **Alexei Bagrets** (Karlsruhe Institute of Technology)
"Kondo effect in binuclear metal-organic molecules on metallic surfaces"
14:40 – 15:00 **Jacob Lykkebo** (University of Copenhagen)
"Strong Overtones Modes en IETS with Cross-Conjugated Molecules"
15:00 – 15:30 Coffee Break
15:30 – 16:10 **Alessandro Pecchia** (CNR-ISMN)
"Current across molecules: pathways, vibrations and heat"
16:10 – 16:50 **Magnus Paulsson** (Linnaeus University)
"Inelastic scattering and conformational change in molecular junctions"

16:50 – 17:00 **Closing remarks**

4. List of posters

#	Title	Presenter
P 1	Kondo effect in binuclear metal-organic molecules on metallic surfaces	Bagrets, Alexei
P 2	First-principles simulation of electron transport in Nanoelectronic devices	Bani-Hashemian, Mohammad Hossein
P 3	Conformational dynamics and steady-state currents: feel the heat	Borges, Anders
P 4	Phonon spectrum modifications in molecular junctions under bias: an ab-initio study	Cucinotta, Clotilde
P 5	Density-Functional Theory with Self-Consistent Long-Range van der Waals Interactions	Ferri, Nicola
P 7	Simulating force and conductance of molecular junctions: A theoretical study	Gross, Lynn
P 8	Mechanically activated molecular devices through single-molecule pulling	Franco, Ignacio
P 9	Current Density vs Vibrations in MTJs	Hansen, Thorsten
P 10	Localized Channel Currents - Elastic and Inelastic Contributions	Hansen, Tim
P 11	Implementation of Smeagol into Fireball DFT code	Hapala, Prokop
P 12	Electron-vibration interactions in charge transport through molecular junctions	Hellmuth, Thomas
P 13	Electronic communication through molecular bridges	Herrmann, Carmen
P 14	Thermopower for molecular chains with exponentially suppressed transmission	Karlström, Olov
P 15	Coherent electron transport in single molecule junctions under electrochemical conditions	Kastlunger, Georg
P 16	Scanning Gate Microscopy of Quantum Dots: Fabry-Pérot Interferences and Thermally Induced Rings	Kleshchonok, Andrii
P 17	Exploring coherent transport through π-stacked systems in molecular electronic devices	Li, Qian
P 18	Benzene strongly adsorbed on metal surfaces: Chemisorption, physisorption, or both?	Liu, Wei
P 19	Strong Overtones Modes in Inelastic Electron Tunneling Spectroscopy with Cross-Conjugated Molecules: a prediction from theory	Lykkebo, Jacob
P 20	Electronic transport through star-shaped Fe4 nanomagnet	Maslyuk, Volodymyr
P 21	Charge transport across insulating self-assembled monolayers: Non-equilibrium approaches and modeling in studies of relation between current and molecular structure	Mirjani, Fatemeh
P 22	Ab Initio Investigations of the Interaction of Imidazole (Im) - CO2 Complexes at Gold Clusters and Surfaces	Muthuramalingam, Prakash
P 23	Quantum pump in molecular motor	Napitu, Berlinson D.

#	Title	Presenter
P 24	Inelastic effects on the electronic current noise through nanojunctions	Novotny, Tomas
P 25	Atomistic modelling of dynamical quantum transport -	Oppenländer, Christian

	admittance and higher harmonics	
P 26	From spin-polarized interfaces to giant magnetoresistance in organic spin valves	Otalvaro, Diana
P 27	Simulating Single-molecule Pulling Experiments	Pirrotta, Alessandro
P 28	Sequential transport through molecules with rapidly fluctuating bridges	Popescu, Bogdan
P 29	Simulation of Quantum Interference & Spin Filtering Properties in Organic Radicals Probed by Mechanical Break Junctions	Renaud, Nicolas
P 30	Density-Functional Theory with Screened van der Waals Interactions for the Modeling of Hybrid Inorganic/Organic Systems	Ruiz Lopez, Victor G.
P 31	Flux densities and tunneling velocities in symmetric double well potentials	Schild, Axel
P 8	Mechanically activated molecular devices through single-molecule pulling	Solomon, Gemma
P 32	Electron hopping transport in single molecule junctions under electrochemical conditions	Stadler, Robert
P 33	Transient dynamics of a molecular junction driven by time-dependent voltage pulses	Zelinskyy, Yaroslav
P 34	Single molecule spectroscopy via generating function approach	Zheng, Yujun
P 35	A Reversible Molecular Switch Based on the Biphenyl Structure	Zoloff Michoff, Martin

5. List of participants

1	Alexei	Bagrets	Germany	alexej.bagrets@kit.edu
2	Mohammad H.	Bani-Hashemian	Switzerland	hossein.banihashemian@mat.ethz.ch
3	Jörg	Behler	Germany	joerg.behler@theochem.ruhr-uni-bochum.de
4	David	Beratan	USA	david.beratan@duke.edu
5	Anders	Borges	Denmark	andersborges@chem.ku.dk
6	Gabor	Csanyi	United Kingdom	gc121@cam.ac.uk
7	Clotilde	Cucinotta	Ireland	c.cucinotta@tcd.ie
8	Gianaurelio	Cuniberti	Germany	g.cuniberti@tu-dresden.de
9	Marcus	Elstner	Germany	marcus.elstner@kit.edu
10	Ferdinand	Evers	Germany	ferdinand.evers@kit.edu
11	Nicola	Ferri	Germany	ferri@fhi-berlin.mpg.de
12	Ignacio	Franco	USA	franco@chem.rochester.edu
13	Michael	Galperin	USA	migalperin@ucsd.edu
14	Marc H.	Garner	Denmark	gpz485@alumni.ku.dk
15	Leonhard	Grill	Austria	lgr@fhi-berlin.mpg.de
16	Lynn	Gross	Germany	grossl@chemie.uni-hamburg.de
17	Thorsten	Hansen	Sweden	Thorsten.Hansen@chemphys.lu.se
18	Tim	Hansen	Denmark	tim.hansen@chem.ku.dk
19	Prokop	Hapala	Czech Republik	ProkopHapala@gmail.com
20	Thomas	Hellmuth	Germany	thellmut@tfp.uni-karlsruhe.de
21	Carmen	Herrmann	Germany	carmen.herrmann@chemie.uni-hamburg.de
22	Josh	Hihath	USA	jhihath@ucdavis.edu
23	Olov	Karlström	Denmark	olov@chem.ku.dk
24	Georg	Kastlunger	Austria	georg.kastlunger@univie.ac.at
25	Andrii	Kleshchonok	France	andrii.kleshchonok@cea.fr
26	Leeor	Kronik	Israel	leeor.kronik@weizmann.ac.il
27	Kasper	Lauritzen	Denmark	KPLauritzen@gmail.com
28	Qian	Li	Denmark	qian.li@chem.ku.dk
29	Wei	Liu	Germany	wliu@fhi-berlin.mpg.de
30	Jacob	Lykkebo	Denmark	jacoblj@chem.ku.dk
31	Dmitrii	Makarov	USA	makarov@cm.utexas.edu
32	David	Masiello	USA	masiello@chem.washington.edu
33	Volodymyr	Maslyuk	Deutschland	volodymyr.maslyuk@physik.uni-halle.de
34	Volkhard	May	Germany	may@physik.hu-berlin.de
35	Fatemeh	Mirjani	Netherlands	F.Mirjani@tudelft.nl
36	Nikolaj	Moll	Switzerland	nim@zurich.ibm.com
37	Prakash	Muthuramalingam	France	prakashspm@gmail.com

38	Berlinson D	Napitu	Netherlands	b.d.napitu@tudelft.nl
39	Tomas	Novotny	Czech Republic	tno@karlov.mff.cuni.cz
40	Christian	Oppenländer	Germany	christian.oppenlaender@physik.uni-regensburg.de
41	Diana	Otalvaro	Netherlands	d.otalvaro@utwente.nl
42	Nacho	Pascual	Spain	ji.pascual@nanogune.eu
43	Magnus	Paulsson	Sweden	magnus.paulsson@lnu.se
44	Alessandro	Pecchia	Italy	alessandro.pecchia@ismn.cnr.it
45	Alessandro	Pirrotta	Denmark	tqn722@alumni.ku.dk
46	Bogdan	Popescu	Germany	b.popescu@jacobs-university.de
47	Nicolas	Renaud	Netherlands	n.renaud@tudelft.nl
48	Michael	Rohlfing	Germany	rohlfin@uni-muenster.de
49	Angel	Rubio	Spain	angel.rubio@ehu.es
50	Victor G.	Ruiz Lopez	Germany	ruiz@fhi-berlin.mpg.de
51	Elke	Scheer	Germany	elke.scheer@uni-konstanz.de
52	Axel	Schild	Germany	axel.schild@fu-berlin.de
53	Gemma	Solomon	Denmark	gsolomon@nano.ku.dk
54	Robert	Stadler	Austria	robert.stadler@univie.ac.at
55	Stefan	Tautz	Germany	s.tautz@fz-juelich.de
56	Alexandre	Tkatchenko	Germany	tkatchenko@fhi-berlin.mpg.de
57	Diana C.	Urbanek	Spain	diana-camila.urbanek@icfo.es
58	Latha	Venkataraman	USA	lv2117@columbia.edu
59	Thomas	Wandlowski	Switzerland	thomas.wandlowski@dcb.unibe.ch
60	Yaroslav	Zelinskyy	Germany	izelinskyi@physik.hu-berlin.de
61	Yujun	Zheng	China	yzheng@sdu.edu.cn
62	Martin	Zoloff Michoff	Germany	martin.zoloff@theochem.ruhr-uni-bochum.de