Ψ_k **Scientific Highlight Of The Month**

No. 128 **October 2015**

2015 Psi-k Conference

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Abstract

We dedicate this issue of the Psi-k Newsletter to the 2015 Psi-k Conference. We provide a brief overview of the conference, some photos of the event, a breakdown of the origins of the conference attendees, and a series of short personal reflections by a few researchers who very kindly took the time to provide their impressions. We also provide a copy of the full scientific program at the end, and include a section about the Volker Heine Young Investigator Award and its associated symposium.

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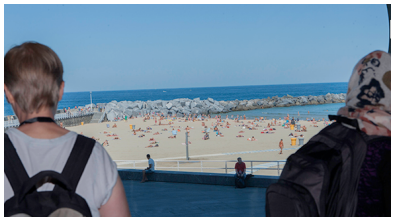
2015 Psi-k Conference
http://nano-bio.ehu.es/psik2015/

6-10 September, 2015
Kursaal Congress Centre, Donostia-San Sebastián, Spain



Conference Overview

The conference was organized by Co-Chairs **Angel Rubio** and **Risto Nieminen**. They were assisted by the staff of the University of the Basque Country, with tremendous logistical support from the local events managers at Ercisa Congresos. We thank the Program Committee members for their valuable help in preparing the program as well as many members of the Psi-k community for their contributions and suggestions.

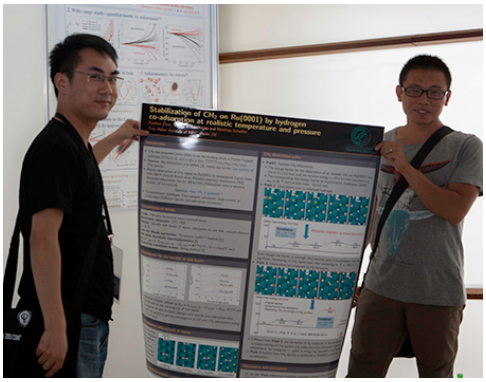
The initial registration period on September 6th was overflowing with eager researchers who collected black bags with white conference logos containing blue event t-shirts, programs, and other items. The weather was unusually sunny and clear for most of the week, and many guests reportedly enjoyed a bit of free time on the beach along the picturesque Bay of Biscay.

The conference was inaugurated by Co-Chairs Angel Rubio and Risto Nieminen, University of the Basque Country Vice-Rector of Research **Fernando Plazaola**, and Vice-Consul of Universities and Research for the Basque Government **Adolfo Moraís**. The speakers were greeted by an award-winning dancer who performed an *aurresku*, a traditional Basque dance to honor guests. The contributions of **Walter Temmerman** to Psi-k and the electronic structure community were acknowledged at the opening ceremony and at a special symposium on f-electrons organized in his memory.

The conference ran very smoothly; all the technicians were very helpful and no major delays were accumulated during the day.

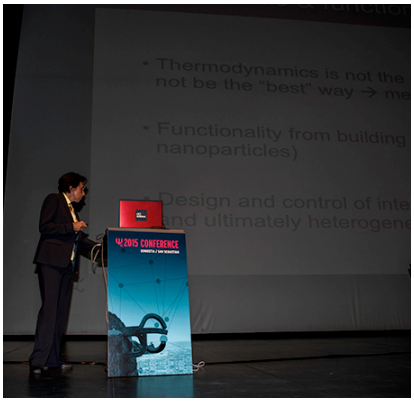
The 2015 edition of the Psi-k Conference was the largest to date, with slightly less than 1,200 registrants and six parallel sessions. There were five plenary talks, 30 symposia, 160 invited speakers, and 180 contributed speakers. Many posters (over 700) were displayed over the course of two sessions with a buffet dinner in the same location for an amiably sociable uproar. The posters were of very high quality and were presented in depth by the participants; all the posters were well-attended.

The symposia that received the most abstract submissions were Materials Design (108), Novel 2D Materials and Heterostructures (72), and Theoretical Spectroscopy (58).



A good atmosphere for discussion was supported by the fact that the dinner was distributed in a *pintxos* format (a regional custom of eating small, artfully-arranged dishes) in all the poster areas.

The plenary talks were very exciting, and they addressed different complementary topics. The quality of the presentations was exceptionally high, which was appreciated by most of the participants, and they triggered many discussions afterward. These sessions covered a range of topics in the field, from materials discovery and design (**Giulia Galli**) to transversal transport coefficients (**Ingrid Mertig**), quasi-2D materials (**Steve Louie**), quantum chemistry methods for condensed matter (**Georg Kresse**) and the structural and thermodynamic complexity of modern materials for industrial applications (**Jörg Neugebauer**).



During the parallel sessions, given the sheer number of simultaneous talks, it was certainly not possible for everyone to attend every talk they wanted to hear, but the intellectual energy involved in so much fruitful discussion over such a short period of time was undoubtedly a great appetite stimulant

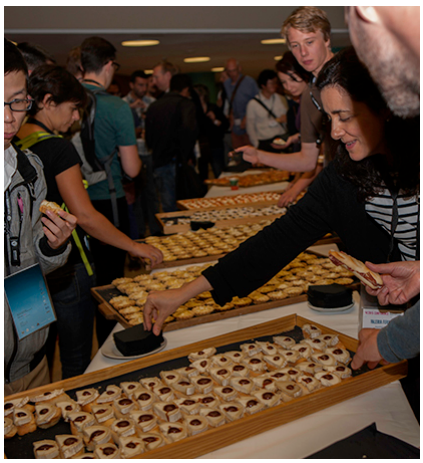
The 2015 Psi-k conference was the third occasion for the presentation of the **Volker Heine** Young Investigator Awards. The purpose of this award is to recognize an individual for her or his outstanding computational work in any type of condensed matter, materials, or nanoscience research involving electronic structure calculations. Five highly talented finalists were selected from a field of 36 very competitive entries. The finalists each presented an excellent thirty-minute talk. An award committee of eight (Risto Nieminen, Matthias Scheffler, Nicola Marzari, and the five plenary speakers) had the difficult task of selecting one winner and four runners-up. The prize winner was **Marco Bernardi** for "Ultrafast Hot Carrier Dynamics in Materials from Ab Initio Calculations." For the 2015 prize, there was one award of 2.500€ and four runner-up prizes of 500€ each, certificates, and a special section for finalist articles in the European Physical Journal B (EPJB, Springer) that will come out in 2016.

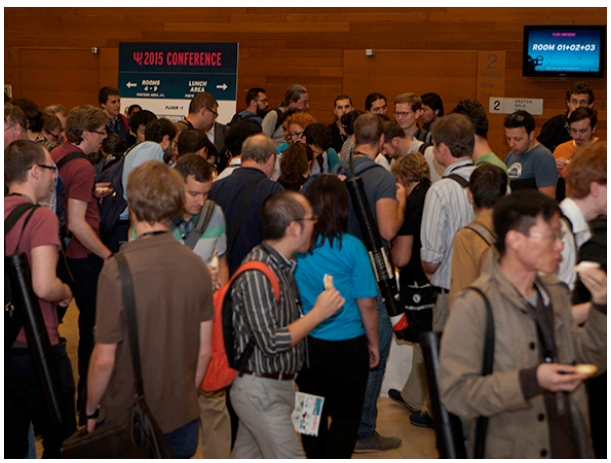
After the Volker Heine award ceremony, there was a brief presentation by representatives from three recently approved EU Centers of Excellence. Risto Nieminen and Angel Rubio introduced the newly recognized centers, which were as follows:

- **Matthias Scheffler**: NoMad
- **Elisa Molinari**: MAX
- **Emilio Artacho**: E-CAM

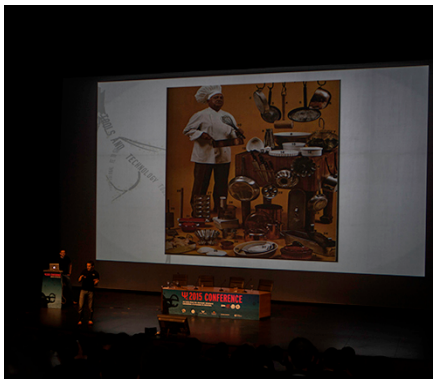
The first two centers will be in operation for three years and the last for five.

The on-site caterer conveniently provided lunch, dinner, and coffee breaks, and guests were treated to a number of local dishes, including squid in ink sauce and *babarrunak* (red beans). Kosher, vegan, and vegetarian meals were available to all who asked. Childcare was provided on site for 12 children of attending researchers, and they all enjoyed their time at the Kursaal.





An underlying gastronomy theme was evident in Wednesday night´s guest talk by **Dani Lasa** and **Ramón Perise** of Mugaritz Restaurant, which is considered to be one of the best restaurants in the world. Lasa and Perise talked about the power of food to evoke emotion and memory, and they discussed their innovative and sometimes winsome approach to creating unparalleled dining experiences through a scientific approach.

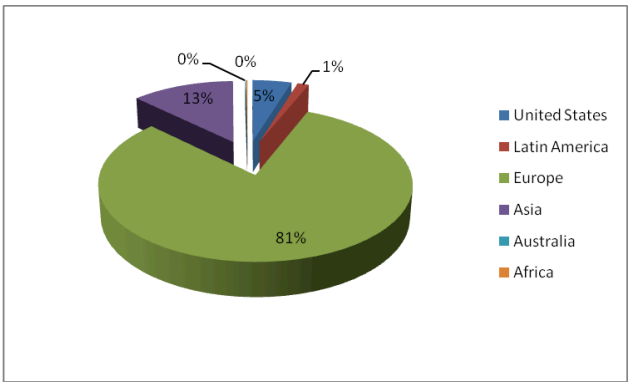


The Gala Dinner took place at two sites, with 700 people at the San Telmo Museum and the others at the Aquarium of San Sebastián, with the spouses of many investigators present as guests. San Telmo is situated in a converted convent, and guests enjoyed an elegant atmosphere accompanied by the *txalaparta* (a Basque percussion instrument used in the past to communicate over long distances) and traditional dances from around the Basque Country. Aquarium guests enjoyed the casual atmosphere among the venue´s beautifully curated exhibits. The dinner began with addresses by Angel Rubio, Fernando Plazaola, San Sebastián Mayor **Eneko Goia**, and Gipuzkoa General Representative **Marko Olano**. Guests enjoyed a wide variety of regional foods and drinks along with the fellowship of their colleagues.

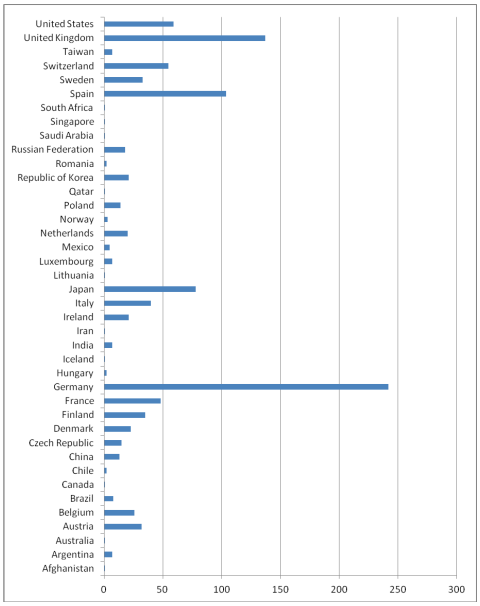
During the closing address, Angel Rubio thanked the organizers and presented a thoughtful and often humorous collection of photos taken during the conference.

A select collection of photos can be viewed at the conference website, at the following link: http://nano-bio.ehu.es/psik2015/photo-album.html.

In terms of attendees, Europe was best represented with 986 guests, as expected. Asia followed with 152 people, followed by the United States, Latin America, Africa, and Australia.



In terms of nationalities, attendees from institutions in 39 countries with origins in 92 different nations were represented. Germany had by far the highest number of representatives, with 242 people, followed by the United Kingdom, Spain, Japan, and the United States. We were fortunate to host a number of attendees from very far away, including Australia, China, Brazil, Chile, Mexico, Afghanistan, and Singapore.



With respect to gender balance, female scientists made up 16% of the total registrants and 13% of the speakers.

There is always room to increase the diversity of conference attendees. Thanks to the generosity of the University of the Basque Country, the Basque Government, the Donostia International Physics Center, the San Sebastián Convention Bureau, the Kursaal, and others, the organizing committee was able to provide financial assistance to 80 attendees.

We wish to thank everyone who attended for their wonderful contributions. Given the high attendance and the positive feedback received from attendees, we consider the conference to have been a success.

Maria-Liesse Doublet said, “I wanted to thank you a lot for your help and the perfect organisation of the meeting. I had a great time.” Of the venue, Giulia Galli wrote, “Thank you all and I'm really sorry to leave San Sebastian, it's just a great place (and the food...my goodness...I thought I would never say that but I have to: better than Italy!!!).”

We wish the organizers of the 2020 conference even greater success.

Personal reflections by conference attendees

“First of all San Sebastián is a lovely location. The Kursaal conference centre is beautiful and the organization was very well done, from the crucial things all the way to the small details.

I congratulate your entire team! “

“From the science point of view the program was nicely done, with a good mix of invited and contributed talks. I come from the experimental world so it was generally hard for me. Nevertheless the quality of the talk looked high, throughout. Only a small percentage of the presenters made the connection with the experimental side of the problem they were researching, which was a pity. But I know in some cases this is a very difficult thing to do. I saw that the program included some topics that go beyond the remit of materials electronic structure. This was interesting. Also it's interesting to see that the disciplines contributing to this topic are not just chemistry, physics, materials science, but also computer science. Perhaps intentional, there was a strong focus on hard cond matt, and interfaces. I don't know if there could be a chance to include more soft materials in the future”.

“The VH session was well attended and the people I spoke with, especially the younger ones, thought it was very cool to have VH around at the conference, even though not everyone knew what he achieved in his time. I would be supportive of creating a link between EPJB and the VH award also in the future editions. I think EPJB could be a vehicle to make this prize more established and known even outside Europe. So maybe what was done at this conference could be the beginning of a happy relationship with mutual benefits. The number of applicants for the award was large enough to allow the selection of 5 really outstanding people. If this award becomes more known internationally and continues to be seen as an opportunity for young researchers to excel and be selected by a competent committee, these are features that EPJB will wish to be associated with, especially as we want to bring the journal to the younger generations. Angel, you have been instrumental in creating the first formula for a EPJB-VH collaboration. I hope that you can continue to put EPJB forward when the future of this prize will be discussed.”

My only (not very important) negative was: the program booklet was printed in a font that was too small (at my age I'm feeling oh so ashamed as I write this!) and didn't contain all the relevant information one needs, like the title of the talks.”
-**Maria Bellantone**, Senior Publishing Editor, Springer

“The Psi-k conference highlighted the mature but at the same time quickly developing electronic structure community in Europe and worldwide.
The talks presented state-of-the-art theoretical developments and the wide ranging class of applications that aim to understand the behavior of real materials. The quick pace of development of the electronic structure field is simply breathtaking. In this regard, the Psi-k conference offered a unique opportunity for both junior and senior participants to digest the current snapshot of theory and applications of first-principles electronic structure methods.

The location -- Kursaal -- offered an optimal way to interact and meet people in the multiple halls and rooms. The many bars and restaurants around Kursaal made the Psi-k conference even more attractive. The unofficial discussions during lunches and dinners were also useful and lead to many new ideas and collaborations. I've established collaborations with two new groups and got several new ideas, which arose during exciting talks and discussions at the conference.

In summary, the Psi-k Conference continues to be at the forefront of electronic structure community worldwide, and Psi-k 2015 in San Sebastian was a real highlight for me and the rest of my group. The feedback from the students and

postdocs in my group has been extremely positive and I feel that the Psi-k conference has helped to get considerable steam for our research during the next 5 years!"
-**Alexandre Tkatchenko**, Fritz-Haber Institute

"Psi-k 2015 was a great success. First it has confirmed the growing recognition of the relevance of atomistic simulations and electronic structure calculations are central to the understanding of diverse domains of science. It has also shown that a great effort is ongoing worldwide in trying both to understand "real" materials and "real" processes and to improve our theoretical and computational schemes. Beyond any doubt, Psi-k 2015 has demonstrated the existence of an enthusiastic community that recognizes itself under the label "Psi-k". Last, but not least, the organization of the Conference was superb. Great choice of the scientific program and of the location (splendid)! Many thanks to Angel and his team, who have now established a new standard for Psik-k conferences to come."
-Wanda Andreoni, EPFL

***Photo credits: Ixone Sadaba**

Acknowledgments:

We are sincerely thankful for the invaluable support of the local administration at the UPV/EHU, in particular Izaskun Ibarbia, Kate Chabarek, and Cecilia Benguria as well as the excellent staff of ERCISA, with special thanks to Nerea Ortiz de Pinedo, Izaskun Ardanaz, and Yolanda Guerediaga. Many thanks to Mugaritz Restaurant for their presentation, which was greatly appreciated by the attendees.

The conference would not have been possible without the support of the Psi-K Organization and the ESF Research Networking Program, "Advanced Concepts in Ab-initio Simulations of Materials" as well as the UPV/EHU, the Basque Government, the Donostia International Physics Center, the Gipuzkoa Provincial Government, the San Sebastián Convention Bureau, the Kursaal, and everyone else who was involved in supporting and organizing the conference. We thank you again for all your support.

MONDAY
SEPTEMBER 7, 2015

PLENARY TALK	SYMPOSIUM	INVITED TALK	CONTRIBUTED TALK	POSTER SESSION

TIME	AUDITORIUM (1.806)	CHAMBER HALL (624)	ROOMS 1+2+3 (575)	ROOM 10 (169)	ROOMS 4+5 (110)	ROOMS 8+9 (100)
08:30	Welcome					
09:00	Plenary 1 Giulia Galli: *Materials discovery and scientific design by computation: what does it take?*					
09:15						
09:30						
09:45	**S1 Thirty Years of Car-Parrinello** Chairs: Michiel Sprik. Giulia Galli. S1 I1 Christian Carbogno: *Accurate Thermal Conductivities from First Principles*	**S19 Materials Design.** Chairs: Nicola Marzari		**S22 Electron Phonon Coupling and Thermoelectricity.** Chairs: Georg Madsen	**S13 Magnetic Excitation and Magnetization Dynamics.** Chairs: Stefan Blügel	
10:00		S19 I1 Kristin Persson: *The Materials Project: Accelerated Materials Design in the Information Age*		S22 I1 Lilia Boeri: *Bonding, Electron-Phonon Interaction and Superconductivity in high-pressure hydrides*	S13 I1 Marco Battiato: *Ultrafast spin injection in semiconductors*	
10:15	S1 C1 Marivi Fernandez-Serra: *First Principles Liquid Water: the quest for the perfect density functional*		**S7 Novel Density Functionals.** Chairs: John Dobson. Robert DiStasio			**S18 Electrochemical Energy Storage and Conversion: Solid/Liquid.** Chairs: Axel Gross. Marie Pierre Gaigeot.
10:30	S1 C2 Federica Agostini. *Coupled electron-nuclear dynamics in non-adiabatic process: The exact factorization approach*	S19 I2 Giovanni Pizzi: *The ADES model and the AiiDA infrastructure for Computational Materials Science*	S7 I1 Neepa Maitra: *Time-Dependent Density Functional Theory For Non-Equilibrium Dynamics : An Exact Condition*	S22 C1 Yannick Gillet. *First-principles study of frequency-dependent Resonant Raman scattering*	S13 C1 Christoph Friedrich. *Acoustic magnons in the long-wavelength limit: resolving the Goldstone violation in many-body perturbation theory*	S18 I1 Marie-Liesse Doublet: Interface Electrochemistry in Li-Materials: A First Step towards Multiscale Modeling
10:45	S1 I2 Robert DiStasio: *The Microscopic Structure, Equilibrium Density, and Local Enviroment of Liquid Water*			S22 I2 Nicola Bonini: Thermoelectric properties from first-principles: electron-phonon interactions and the Boltzmann transport equation	S13 C2 Jacopo Simoni. *Ultrafast magnetism within Time Dependent Density Functional Theory*	
11:00		S19 C1 Stefaan Cottenier: *Bringing DFT codes back to the testbench: what did we learn?*	S7 C1 Paul Erhart: *A variational polaron self-interaction corrected total-energy functional for charge excitations in insulators*		S13 I2 Hardy Gross: *Ultrafast laser-induced demagnetization of ferromagnetic solids*	S18 C1 Javier Carrasco: *Ion insertion into layered transition metal oxides for batteries: Insight from van der Waals density functional*
11:15	S1 C3 Mariana Rossi. *Nuclear Quantum Effects in the Dynamics of Biologically Relevant Systems from First Principles*	S19 C2 Christoph Schober. *Efficient first-principles based screening for high charge carrier mobility in organic crystals*	S7 C2 Ute Werner: *Local versus Non-Local Exact Exchange in Hybrid Functionals*	S22 C2 Roman Kovacik: *Spin transport and spin-caloric effects in (Cr,Zn)Te half-metallic nanostructures: Effect of spin disorder at elevated temperatures from first principles*		S18 C2 Giuseppe Fisicaro: *A Generalized Poisson and Poisson-Boltzmann solver in wet-environments electronic-structure calculations*
11:30	S1 C4 Marco Cazzaniga: *Ab-initio molecular dynamics simulation of polaron- and exciton-OLED degradation*	S19 I3 Richard Needs: *Structure searching and anharmonic vibrations*	S7 I2 Florian Eich: *Noncollinear magnetism in Spin-Density-Functional Theory*	S22 I3 Claudia Draxl: *Aspects of electron-vibrational coupling in electronic-structure theory*	S13 C3 Leonid Sandratski. *Exchange splitting of surface and bulk electronic states in excited magnetic states of Gd: relation to femtosecond-scale pump-probe experiments.*	S18 I2 Adam Foster: *Probing molecular processes at water-insulator interfaces*

11:45	S1 I3 Wanda Andreoni: *Capture of CO2 in Amine Aqueous Solutions: Insights from Ab Initio Molecular Dynamics.*				S13 C4 Ehsan Barati. *Calculation of Gilbert damping and nonadiabatic spin-transfer torque in magnetic nanostructures*	
12:00		S19 I4 Georg Madsen: *High-throughput search for efficient thermoelectrics*		S22 C3 Matthieu Verstraete. *There is no such thing as a simple metal*	S13 I3 Johannes Lischner: *First-principles theory of electron-spin fluctuation interactions in materials*	S18 C3 Anoop Kishore Vatti. *Formation Energy of Halide ions (Cl/Br/I) in water from ab-initio Molecular Dynamics*
12:15	S1 I4 François Gygi: *Verification and Validation of First-Principles Molecular Dynamics Simulations*			S22 I4 Gianni Profeta: *Prediction of Electron-Phonon driven superconductivity: some examples*		
12:30		S19 C3 Thomas Archer: *Which Heusler Alloy distorts?*			S13 I4 Samir Lounis: *Dynamical magnetic excitations of itinerant nanomagnets*	
12:45		S19 C4 Maximilian Amsler: *Novel low-density silicon allotropes for photovoltaic applications*		S22 C4 Kurt Stokbro. *Electron-phonon interactions from first-principles in bulk- and device structures*		
13:00						
13:15	LUNCH		LUNCH			
13:30						
13:45		LUNCH		LUNCH	LUNCH	LUNCH
14:00						
14:15	Plenary 2 Ingrid Mertig: *Transversal transport coefficients and topological properties*					
14:30						
14:45						
15:00	S1 I5 Jürg Hutter: *MP2 and RPA calculations of liquid water*	S19 C5 Federico Calle-Vallejo. *Fast and rational design of multifaceted catalysts by means of structure-sensitive scaling relations*	S7 I3 Paola Gori-Giorgi: *Functionals from the strong-coupling limit of DFT: promises and challenges*	**S14 Chiral Magnetism.** Chairs: Stefan Blügel S14 I1 Stefan Heinze: *Tailoring magnetic skyrmions at transition-metal interfaces*	**S9 DFT for Coupled Matter-Photon Systems.** Chairs: Heiko Appel S9 I1 Heiko Appel, Michael Ruggentaler: *Quantum Electrodynamical Density-Functional Theory: An approach to the time-dependent matter-photon problem*	
15:15		S19 I5 Thomas Bligaard: *Computational catalyst search and validation*				S18 C4 Philipp Pedevilla. *Ab initio molecular dynamics simulations of the water feldspar interface*
15:30	S1 I6 Heather Kulik: *Challenges and advances for accurate large-scale electronic structure and dynamics*		S7 I4 Per Hyldgaard: *On the general-purpose nature of van der Waals density functionals*	S14 C1 Takashi Koretsune. *First-principles study of DM interaction in Mn1-xFexGe*	S9 I2 Kay Dewhurst: *Kohn-Sham equations for ground state and time-dependent density functional theory of quantum electrodynamics*	S18 I3 Axel Gross: *Structure of electrochemical interfaces for energy storage studied from first principles*
15:45		S19 I6 David Vanderbilt: *Theoretical search for realizations of the quantum anomalous Hall state*		S14 C2 Alessandro Stroppa. *First-principles approach to M-nitronyl nitroxide (M = Co, Mn) spin helices*		
16:00	S1 C5 Igor Poltavsky: *Converged Nuclear Quantum Statistics from Semiclassical Path Integral Molecular Dynamics*		S7 C3 Rickard Armiento. *The AK13 exchange functional and beyond*	S14 I2 Yuriy Mokrousov: *Berry phase effects in chiral magnets from first-principles theory*	S9 C1 Mehdi Farzananehpour: *Quantum electrodynamical time dependent density-functional theory for many-electron systems on a lattice*	S18 I4 Michiel Sprik: *Supercell modelling of charged oxide electrolyte interfaces*

16:15	S1 I7 Michele Ceriotti: *Generalized Langevin Equations: Fine-tuning Molecular Dynamics from Car-Parrinello, to Efficient Sampling, to Quantum Effects*	S19 C6 Boris Kozinsky. *Design and screening of ionic and electronic conductors for energy application using new approximations and automation.*	S7 I5 Karsten Jacobsen: *Bayesian Error Estimation Functionals*		S9 I3 Eberhard Engel: *Electron-Photon Coupling in Stationary Relativistic DFT*	
16:30		S19 I7 Chris Wolverton: *Materials Genome Approach to Computational Design of Nanostructured Thermoelectrics*		S14 C3 Maia Vergniory. *Spin-texture induced by oxygen vacancies in SrTiO3 (001) surface by first-principles*		S18 C5 Tilde Cucinotta. *The electrostatic double layer of Pt/water interfaces from first principles molecular dynamics*
16:45	S1 I8 Angelos Michelides: *Water at interfaces and other hydrogen bonded systems – insight from ab initio molecular dynamics*		S7 C4 Kati Finzel: *Shell structure based functionals for the kinetic energy*	S14 I3 Manuel Pereiro: *Topological excitations in a chiral kagome magnet*	S9 C2 Johannes Flick: *Kohn-Sham Approach to Cavity QED: Exact vs. Approximate Effective Fields*	S18 I5 Mira Todorova: *Electrochemistry from the perspective of semiconductor defect chemistry: New tools and insights*
17:00		S20 Machine Learning Methods in Materials Modeling (partial). Chairs: Gabor Csanyi. Alexandre Tkatchenko S20 I1 Luca Ghiringhelli: *Learning descriptors from (big) data: robustness and causality*	S7 C5 Peter Elliott: *Almost exact exchange at almost no computational cost*		S9 I4 Robert van Leuuwen: *Kadanoff-Baym equations for time-dependent coupled electronboson systems*	
17:15	S1 C6 Biswajit Santra: *Predicting anomalous properties of water using ab initio molecular dynamics*		S7 I6 Alexandre Tkatchenko: *Quantum Fluctuations and Non-Covalent Interactions in Density-Functional Theory*	S14 C4 Manuel dos Santos Dias: *Spin dynamics of spin-orbit coupled dimers on Pt(111)*		S18 I6 Enge Wang *Water Study at Surface and Interface*
17:30	S1 I9 Minoru Otani: *Electrochemical systems simulated by First-principles molecular dynamics simulations*	S20 C1 Felipe Canova.: *Molecular Network for Lubricant Optimisation*		S14 I4 Laszlo Udvardi: *Finite temperature behavior of spin-spirals and skyrmions*	S9 C3 Camilla Pellegrini: Optimized Effective Potential for Quantum Electrodynamical Time-Dependent Density-Functional Theory	
17:45		S20 C2 Thomas Hammerschmidt. *Robust crystal-structure prediction with structure maps*			S9 C4 Walter Tarantino. *Extended Kohn-Sham Systems for Quantum Electrodynamical Time-Dependent Density Functional Theory*	S18 C6 Guido von Rudorff. *Structure and charge transfer at the hematite(001)-water interface from all-QM DFT molecular dynamics*
18:00	S1 C7 Bernd Meyer: *Proton transfer dynamics at the solid/liquid interface*	S20 I2 Anatole von Lilienfeld: *Machine Learning Methods for the Rapid Yet Accurate Sampling of Chemical Compound Space*			S9 I5 Ivano Tavernelli: *Nonadiabatic dynamics with relativistic effects*	S18 I7 Kevin Leung: *Modeling the Voltage Dependence of Electrochemical Reactions at Solid-Solid and Solid-Liquid Interfaces in Batteries*
18:15	S1 I10 Annabella Selloni: *Electrons and holes at the TiO2 water interface*					
18:30						
18:45	DINNER AND POSTER SESSION 1 Dinner will be available between 18:30 and 20:30. Posters should be up not later than 13:00. Authors are expected at their posters between 18:30 and 21:30. Authors presenting their posters on Monday should remove their presentations before 10:00 on Tuesday.					
22:00						

TUESDAY
SEPTEMBER 8, 2015

PLENARY TALK | SYMPOSIUM | INVITED TALK | CONTRIBUTED TALK | POSTER SESSION

TIME	AUDITORIUM (1.806)	CHAMBER HALL (624)	ROOMS 1+2+3 (575)	ROOM 10 (169)	ROOMS 4+5 (110)	ROOMS 8+9 (100)
09:00	Plenary 3 Steve Louie: *Novel Interaction and Correlation Effects in Quasi 2D Materials*					
09:15						
09:30						
09:45	**S4 Correlated Electrons.** Chairs: Markus Aichhorn	**S20 Machine Learning Methods in Materials Modeling** (cont'd). Chairs: Gabor Csanyi. Alexandre Tkatchenko	***Volker Heine Award***			**S27 Transport Properties.** Chairs: Hardy Gross
10:00	S4 I1 Gianluca Giovannetti. *What about "Ferroelectric Metals" ?*	S20 I3 Joerg Behler *Neural Network Potentials for Large-Scale Molecular Dynamics Simulations*	Fabio Caruso. *Comprehensive material modelling within the GW approximation*	**S12 Spin-Orbit Coupling Effects in First-Principles Quantum Transport.** Chairs: Silvia Picozzi	**S2 GW and BSE.** Chairs: Olivia Pulci. Friedhelm Bechstedt y Matteo Gatti.	S27 I1 Stefan Kurth: *Steady-state density functional theory for finite bias conductances*
10:15						
10:30	S4 C1 Yusuke Nomura. *Non-empirical calculation of transition temperature for alkali-doped fullerene superconductors*	S20 C3 Atsuto Seko. *First principles interatomic potentials via compressed sensing*	Ion Errea: *Efficient ab initio calculation of anharonic properties in solid.*	S12 I1 Frank Freimuth: *Transverse transport properties and spin-orbit torques from first principles*	S2 I1 Silke Biermann: *From LDA++ to X+DMFT: strategies for interfacing electronic structure and many-body theory*	S27 I2 Jeff Neaton: *Tunneling and Diffusive Charge Transport at the Nanoscale from First Principles*
10:45	S4 C2 Ryosuke Akashi. *Density Functional Theory for Plasmon-Assisted Superconductivity: Development and Its Applications*	S20 C4 Matthias Rupp. *Quantum Mechanical Properties of Atoms in Molecules via Machine Learning*				
11:00	S4 C3 Michele Casula: *From dynamically screened Hubbard U to Holstein phonons in extended dynamical mean-field theory*	S20 I4 Gabor Csanyi: *Bridging the GAP: fitting first principles potential energy surfaces systematically*	Marco Bernardi. *Ultrafast Hot Carrier Dynamics in Materials from Ab Initio Calculations.*	S12 C1 Guang-Yu Guo: *Anomalous Hall effect and current spin polarization in Co-based Heusler compounds*	S2 C1 Emanuele Maggio: *Bethe-Salpeter equation for correlation energies and post-GW self-energies*	S27 C1 Colin Van Dyke: *Molecular Rectifiers: A new design based on asymmetric anchoring moieties*
11:15	S4 I2 Luca De Medici: *A review of recent experimental evidences of (orbital-selective) Mott physics in Iron Superconductors*			S12 C2. Nicolae Atodiresei: *Organic-Ferromagnetic Spin-Valve Effect*	S2 C2 Wei Chen. *Accurate band gaps of extended systems via efficient vertex corrections in GW*	S27 C2 Gianluca Stefanucci: *Transient quantum transport: Nonequilibrium Green's Function Approach Made Fast*
11:30		S25 C1 Daniele Passerone. *Electronic and Optical Properties of Atomically Precise Graphene Nanoribbons and Heterojunctions*	Andreas Grüneis. *Expanding the scope of wave function based methods for solids*	S12 I2 Martin Gradhand: *Spin and Charge Hall effects as a tool for the characterisation of Complex Materials*	S2 I2 Antonio Sanna: *Ab-initio superconductivity: SCDFT and Eliashberg*	S27 I3 Giovanni Vignale: *Time-dependent thermoelectric transport at the nanoscale*
11:45	S4 C4 Ambroise van Roekeghem *Spectral properties of transition-metal pnictides: non-local exchange and dynamical screening*					

12:00	S4 I3 Philipp Hansmann: *Probing materials on different timescales: Fast spectroscopy vs. slow microscopy*	LUNCH	Johanna Fuks: *Time - Resolved Spectroscopy in Time - Dependent Density Functional Theory: An Exact Condition*	S12 C3 Søren Smidstrup: *Nonequilibrium spin density in current-carrying topological insulator thin film*	S2 C3 Arjan Berger: *Fully parameter-free calculation of optical spectra for insulators, semiconductors and metals from a simple polarization functional*	S27 C3 Rajarshi Tiwari. Modeling electronic transport in layered organic crystals
12:15				S12 C4 Jakub Zelezny: *Spin-Orbit Torque in Antiferromagnets*	LUNCH	S27 C4 Giorgia Fugallo. *Thermal Conductivity of Graphene and Graphite: Collective Excitations and Mean Free Paths*
12:30	S4 C5 David Jacob: *NanoDMFT: First principles description of strongly correlated electrons in molecular devices*		LUNCH	LUNCH		S27 I4 Chun Zhang: *Ab initio modeling of steady-state transport properties of nonequilibrium quantum systems*
12:45	S4 C6 Peitao Liu: *Electronic, magnetic and optical properties of Sm+1lrnO3n+1 (n=1, 2, and infinity)*					
13:00	LUNCH					
13:15		**S25 Novel 2D Materials and Heterostructures.** Chairs: Kristian Thygesen				
13:30		S25 I1 Geert Brocks *Interactions and charge transfer in heterostructures of 2D materials*				LUNCH
13:45		S25 C2 Lede Xian and Seymur Cahangirov: *The atomic and electronic structure of silicene and germanene on substrates*				
14:00		S25 I2 Mei-Yin Chou: *Interplay of Charge and Lattice Distortion in Monolayers of Transition Metal Dichalcogenides*			S2 C4. Andrea Ferretti: *Electron and Optical Spectroscopies of Graphene Nanoribbons on Au(111): Insights from Ab-Initio Calculations*	
14:15					S2 I3 Mark van Schilfgaarde: *How well does \emph{GW} Describe Magnetism?*	
14:30	S4 I4 Alessandro Toschi: *Quantum many-body theory at the twoparticle level: The new frontier*	S25 C3 Jacek Majewski: *Multi-scale studies of group IV honeycomb layers and their binary alloys*	**S15 First-Principles Calculations for Multiferroics and Magnetoelectrics.** Chairs: Silvia Picozzi			
14:45		S25 C4 Andrea Cepellotti: *Phonon hydrodynamics and second sound in 2D materials*	S15 I1 Eric Bousquet: *First-principles study of magnetoelectricity: finite magnetic field and density functional perturbation theory.*		S2 C5 Carina Faber: *GW for Electron-Phonon Coupling Calculations in Carbon-based Materials*	
15:00	S4 I5 Alexey Rubtsov: *The dual-boson description of collective modes in correlated systems*	S25 I3 Arkady Krasheninnikov: *Defects in two-dimensional materials: their production under irradiation, evolution and properties from first-principles calculations*	S15 C1 Zeila Zanolli: *Magnetoelectric multiferroic superlattices and interfaces*	S12 I3 Qian Niu: *Orbital Magnetism and Landau Levels*	S2 C6. Jens Wehner. *Multiscale simulation of exciton diffusion in organic materials via GW-BSE*	**S8 Recent Developments in Density Matrix Functional Theory.** Chairs: Heiko Appel
15:15			S15 C2 Kunihiko Yamauchi: *Rashba splitting and spin-valley coupling in ferroelectric oxides*		S2 C7 Michiel van Setten: *High throughput GW*	S8 I1 Dieter Bauer: *Time-dependent renormalized natural orbital theory for laser-driven correlated few-body quantum dynamics*
15:30	S4 C7	S25 C5 Marco Gibertini: *Engineering polar discontinuities in 2D honeycomb lattices*	S15 I2 Lars Nordstrom: *Ordered space- and time-odd multipoles and their relevance in magneto-electrics*	S12 I4 Diemo Koedde-ritzsch: *Electronic and spin transport within the Kubo Formalism – a relativistic Green function KKR approach*	S2 C8 Deyu Lu: *A local representation of the dielectric response function*	S8 C1 Klaas Giesbertz: *Invertibility of retarded response functions for Laplace transformable potentials: application to one-body reduced density matrix functional theory*

15:45	S4 I9 Eva Pavarini *Origin of orbital-ordering and orbital-order melting transitions in strongly correlated systems*	S25 C6 Alexander Rudenko: *Toward realistic description of black phosphorus: from GW approximation to large-scale modeling*			S2 I5. Francesco Sottile. *Exciton Dispersion from first principles*	S8 C2 Nektarios Lathiotakis *Local potentials in the Reduced Density Matrix Functional Theory: Hybrid DFT-RDMFT approaches*
16:00		S25 I5 Esa Räsänen: *Dirac physics in artificial graphene*	S15 C3 Kun Cao: *Theory of electromagnons in CuO*	S12 C5. Valentina Brosco. *Transport signatures of strong spin-orbit coupling in two-dimensional materials*		S8 C3 Mario Piris. *Towards an N-representable 1-RDM Theory*
16:15	S4 C8 Guoren Zhang: *Fermi surface of Sr2RuO4: Role of anisotropic Coulomb interaction and Coulomb-enhanced spin-orbit coupling*		S15 C4 Michael Fechner. *Orbital currents in CuO*	S12 I5 Jairo Sinova: *Relativistic torques in ferromagnets and antiferromagnets*	S2 C9 Iurii Timrov: *Electron Energy Lossand Ineslastic X-Ray Scattering Cross Sections from Time - Dependent Density - Functional Perturbation Theory*	*S8 I2 Sangeeta Sharma: Spectrum within Reduced Density Matrix Functional Theory: application to transition metal oxides*
16:30	S4 C9 Oleg Peil: *A low-energy description of rare-earth nickelates*	S25 C7 Kirsten Winther. *Efficient scheme for calculating the dielectric properties of van der Waals heterostructures*	S15 C5.Takahiro Shimada. *Low-dimensional Atomic Multiferroics: Defects in Nonmagnetic Ferroelectric PbTiO3*		S2 C10 Dmitrii Nabok: *Accurate GoWo quasiparticle energies from FLAPW calculations*	
16:45	S4 I7 Andy Millis: *Many-Body Physics of Materials: Density Functional Plus Dynamical Mean Field and Beyond*	S25 C8 Domenico Di Sante. *Emergence of ferroelectricity and spin-valley properties in twodimensional honeycomb binary compounds*	S15 I3 Massimiliano Stengel: *Flexoelectricity from density-functional perturbation theory*	S12 C6 Libor Smejkal. *Magnetotransport in Disordered Antiferromagnets from First Principles*	S2 C11 Michael Rohlfing: *Tuning the optical spectrum of carbon nanotubes by the environment*	S8 C4 Iris Theophilou. *Generalized Pauli constraints: do they have an effect on Reduced Density Matrix Functional Theory minimization*
17:00		S25 I6 Matteo Calandra: *Universal enhancement of superconductivity in two dimensional semiconductors at low doping by electron-electron interaction*		S12 I6 Zhe Yuan: *Spin transport and relaxation in magnetic heterostructures: the effects of spin-orbit interaction, noncollinear magnetization and finite temperature*		S8 C5 Julius Rapp. *Exact treatment of 3D He in linearly polarized laser fields using TDRNOT*
17:15	S4 I8 Jan Tomczak: *Thermoelectricity and electron-phonon coupling in correlated narrow-gap semiconductors*					S8 I3 Ralph Gebauer: *A favorably-scaling natural-orbital functional theory based on higher-order occupation probabilities*
17:30		S25 C9 Yoshiyuki Miyamoto: *Photo-induced dynamics in low dimensional materials: strong IR illumination inducing lattice and electronic dynamics*				
17:45	S4 C10 Matteo Cococcioni: *Charge localization and energetics of LI-ion batteries cathodes from Hubbard-corrected DFT functionals*	S25 C10 Marcin Szyniszewski. *Diffusion Monte Carlo Study of Charge Career Complexes in Two-Dimensional Semiconductors*				
18:00	S4 I9 Martin Eckstein: *Nonequilibrium dynamical mean-field theory*	S 25 I7 Tony Low: *Aspects of electrons and plasmons propagation in black phosphorus*				
18:15						
18:30	DINNER AND POSTER SESSION 2 Dinner will be available between 18:30 and 20:30. Posters should be up not later than 13:00. Authors are expected at their posters between 18:30 and 21:30. Authors presenting their posters on Tuesday should remove their presentations before 10:00 on Thursday.					
18:45						
22:00						

WEDNESDAY
SEPTEMBER 9, 2015

PLENARY TALK | SYMPOSIUM | INVITED TALK | CONTRIBUTED TALK

TIME	AUDITORIUM (1.806)	CHAMBER HALL (624)	ROOMS 1+2+3 (575)	ROOM 10 (169)	ROOMS 4+5 (110)	ROOMS 8+9 (100)
09:00	Plenary 4 Georg Kresse: *Quantum chemistry methods for condensed matter: current status and future developments*					
09:15						
09:30		**S10 Applications of Quantum Monte Carlo Methods.** Chairs: Matthew Foulkes. Shiwei Zhang	**S11 Upscaling Electronic Structure: Reduced-Scaling and Multi-Scale Methods** **Peter Haynes.** Chairs: Matthias Scheffler	**S16 Ab Initio Statistical Mechanics.** Chairs: Luca Ghiringhelli		**S3 f-electrons.** Chairs: Silke Biermann
09:45						S3 I1 Julie Staunton: *Magnetic ordering and magnetic interactions in rare earth materials described by an ab-initio electronic structure theory*
10:00		S10 I1 Ethan Brown: *Attacking the sign problem in path integral Monte Carlo from two directions*	S11 I1 Lin Lin: *Fast algorithms for Kohn-Sham density functional theory*	S16 I1 Tilmann Hickel *Coupling of magnetic and lattice degrees of freedom in real Materials.*		
10:15	**S6 Recent Advances in Diagrammatic Methods for the Total Energy.** Chairs: Georg Kresse. Patrick Rinke				**S24 Non-Linear Optics of Materials and Nanoplasmonics.** Chairs: Valerie Veniard	S3 C1 Leon Petit. *First principles study of valence and structural transitions in rare earth compounds under pressure*
10:30	S6 I1. Andreas Görling. *Kohn-Sham methods based on the adiabatic-connection fluctuation-dissipation theorem*	S10 I2 Ronald Cohen: *Quantum Monte Carlo for Materials at High Pressures*	S11 C1. Nicholas Hine. *Excited state calculations and theoretical spectroscopy of complex nanomaterials using Linear-Scaling Density Functional Theory*	S16 C1 Sergey Pogodin: *Ab initio Kinetic Monte Carlo study of temperature-programmed desorption spectra of RuO2*	S24 I1 Stefano Corni: *Molecular and nanoplasmonics by first-principle based approaches*	S3 C2 Gertrud Zwicknagel: *Heavy quasiparticles in YbRh2Si2: High temperatures and magnetic fields*
10:45			S11 I2 Luigi Genovese: *The flexibility of Daubechies wavelets for Linear Scaling DFT calculations*	S16 C2 Xunhua Zhao: *Formation of 1D adsorbed water structures on CaO(001): A first-principles genetic algorithm study*		S3 I2 Alexander Shick: *Unified picture of electron correlation effects in unconventional Pu-based superconductors and δ-Pu*
11:00	S6 C1 John Dobson: *Layer Response theory for semi-analytic energetics of vdW bound layered materials*	S10 C1 Ching-Ming Yei: *The Quantum Monte Carlo studies of interactions in van der Waals bilayer systems*		S16 I2 Roberto Car *Free energies and phase diagrams.*	S24 I2 Pablo Garcia (with FJ Vidal): First-principles nanoplasmonics: Plasmon hybridization and photoinduced currents	
11:15	S6 C2. Markus Betzinger: *All-electron RPA total energies with infinite band summations*	S10 C2 Ryo Maezono *Electron Correlation on DNA Stacking: A Quantum Monte Carlo Study*	S11 C2. Pablo Garcia Fernandez. *A systematically improvable second-principles method including electron and lattice degrees of freedom*			S3 I3 Leonid Pourovskii: *Orbital transition and pressure evolution of the low-energy electronic structure in CeM2X2 heavy-fermion superconductors*
11:30	S6 I2 Fred Manby. *Distinguishable Cluster Theory*	S10 I3 Elif Ertekin: *Bulk and defect properties of semiconductors via fixed node diffusion Monte Carlo*	S11 I3 Cedric Weber: *An implementation of dynamical mean field theory for nano-structures and molecules*	S16 I3 Alessandro de Vita: *Molecular Dynamics with On-The-Fly Machine Learning of QM Forces*	S24 C1 Daniel Sanchez: *First-principles calculation of plasmonic near-fields: reaching atomic-scale resolution in nanooptics*	
11:45					S24 C2 Katsuyuki Nobusada: *Optical Response Derived from Electric Field Gradient Inherent in Optical Near Field*	S3 I4 Xi Dai: *LDA+Gutzwiller method and its application to f electron materials*

12:00	S6 C3 Alberto Ambrosetti. *Wavelike Nature of van der Waals Interactions at the Nanoscale*	LUNCH	S11 C3. Shunsuke Yamada: *A new method for calculating one-electron energy spectrum of a large system based on a first- principles divide-and-conquer method*	LUNCH	S24 C3 Lauri Lehtovaara: *Plasmon resonances in monolayer-protected metal nanoparticles*	
12:15	S6 C4 Dario Roca. *Dielectric matrix formulation of correlation energies within the Random Phase Approximation: Inclusion of screened exchange effects*		S11 C4 Arash Mostofi: *Multi-scale theory and simulation of the conductivity of carbon nanotube networks*		LUNCH	S3 C4 Jordan Bieder: *Second-principles atomic potentials for finite temperature simulations: application to SrRuO3 electrode material*
12:30	LUNCH		LUNCH			S3 I5 Nicola Lanata: *Electron Correlations in Plutonium and the Actinides Transition*
12:45						
13:00						S3 C5 Priyanka Seth. *Towards a first-principles determination of effective Coulomb interactions in correlated electron materials: Role of intershell interactions*
13:15						LUNCH
13:30				S16 I4 Ralf Drautz: *Analytic bond-order potentials: from a simplified description of the electronic structure to structural stability in elements and compounds*		
13:45		S10 I4 Sandro Sorella: *Ab-initio molecular dynamics by quantum Monte Carlo*				
14:00	S6 I4 Xinguo Ren: *Renormalized perturbation theory for total and self energies based on diagrammatic techniques*			S16 I5 George Booth: *Sampling, Embedding and Optimizing tractible many-electron wavefunctions in the solid state*		
14:15		S10 C3 Yasmine S. Al-Hamdani. *Using quantum Monte Carlo for the interaction of water with carbonaceous and BN based substrates and assessing exchange-correlation functionals*	S11 I4 Daniel Berger *The QM/MM embedded cluster approach: exploiting locality effectively*			
14:30	S6 C4 Igor Zhang: *Test set for materials science and engineering*	S10 C4 Can Ataca. *High throughput quantum Monte Carlo calculations of material formation energies*		S16 C3. Chiara Panosetti. *Get real! Towards structure prediction of complex systems with efficient global optimization in an ab initio thermodynamics framework*	S24 I3 Alberto Castro *Progress in the theory of control of electron dynamics*	
14:45	S6 I5 Thomas Olsen: *Total energy calculations beyond the Random Phase Approximation*	S10 I5 Leonardo Guidoni: *Structures and properties of (bio)molecules from Quantum Monte Carlo*	S11 C5 Vanessa Jane Bukas: *"Hot" adatoms hopping: Phononic dissipation & equilibration dynamics from first-principles*	S16 I6 Olle Hellman: *Effective lattice dynamics for strongly anharmonic systems*		**S23 Ultrafast Charge Transfer at the Nanoscale.** Chair: Robert van Leeuwen. Gianluca Stefanucci.
15:00			S11 I5 Karsten Reuter *First-Principles Kinetic Monte Carlo for Surface Catalysis: From Exploratory Tool to Commodity*		S24 C4 Tuomas Rossi: *Quantum plasmonics of stretched nanorods*	S23 I1 Oleg Prezdho: *Excited State Dynamics in Nanoscale Materials: A Time-Domain Ab Initio Perspective*
15:15	S6 C6 Jiangqiang Zhou: *Alternative routes for calculations of total energies*	S10 I6 Lucas Wagner: *Understanding strongly correlated systems using quantum Monte Carlo*		S16 C4. Robert Baldock. *Calculating pressure-temperature phase diagrams of materials*	S24 I4 Stefano Ossicini: *Second-order nonlinear optical spectroscopy: theory and applications*	S23 C1 Andrea Marini: *A new approach to describe out-of-equilibrium processes in realistic materials based on the merging of Density-functional Theory with Many-Body Perturbation Theory*

15:30	S6 C7. Christopher Patrick: *Investigating the initial Hamiltonian dependence of non-self-consistent calculations of RPA correlation energies*		S11 C6 Marco Micciarelli: *A multi-scale protocol for simulating the optical properties of natural dyes in solution*	S16 C5. Markus Eisenbach. *Replica Exchange Wang Landau Sampling for First Principles Multiple Scattering Calculation*		S23 C2 Daniele Fazzi. *Modeling ultrafast exciton deactivation and charge transfer processes in organic photovoltaic materials: a chemical physical perspective*
15:45	S6 I5 Garnet Chan. *Quantum chemistry in the condensed phase*	S10 I7 Shiwei Zhang: *Electronic structure calculations in correlated materials: an auxiliary-field perspective*	S11 C7 Jordan Bieder. *Second-principles atomic potentials for finite temperature simulations: application to SrRuO3 electrode material*	**S29 Electronic Structure Theory for Biophysics (partial)** Chair: Leonardo Guidoni S29 I1 Jochen Blumberger: *Electron flow through bacterial nanowire proteins*	S24 C5 Christine Giorgetti: *Ab initio local field effects for surface second harmonic generation*	S23 I2 Carlo Rozzi: *Ultrafast dynamics in light-harvesting and photovoltaics: a theoretical and experimental investigation*
16:00			S11 I6 Dallas R. Trinkle: *Automating diffusivity calculations for interstitial and solute diffusion from first-principles*		S24 C6 Claudio Attaccalite: *Nonlinear reponse of solids within the GW plus Bethe Salpeter approch: application to second and third-harmonic generation*	
16:15	S6 C8 Salih Akbudak. *Numeric atom-centered orbital basis set with correlation consistency for 3d transition metals*	S10 C7 Kayahan Saritas. *Characterizing Physical Errors in DFT for Ring Opening Isomerizations using Quantum Monte Carlo Calculations*		S29 C1. Daniel Cole: *Applications of Large-Scale Electronic Structure Calculations in Biology*	S24 I5 Kazuhiro Yabana: *Time-dependent density functional theory for extreme nonlinear optics*	S23 C3 Elham Khosravi: *Charge-resonance enhanced ionization beyond the quasistatic model: insights from the exact factorization approach*
16:30		S10 I8 Ali Alavi: *Recent developments in FCIQMC*	S11 C8 Eoin O'Reilly: *Multiscale approach to treating random alloy effects in III-N nano structures*	S29 C2. Wei Fang: Nuclear Quantum Effects on the stability of DNA base pairs		S23 C4 Samuel Murphy: Ultrafast laser induced solid-solid phase transitions in tungsten
16:45			S11 I7 Bill Curtin: *X-Mechanics for Flow and Ductility in Metal Alloys*	S29 I2 Carsten Baldauf: *Methods to study and represent the potential-energy surface (PES) of biomolecules in isolation*		S23 C5 Enrico Perfetto: *NEGF approach to pump-probe photoabsorption spectroscopy*
17:00						S23 C6 Jacob Spencer: *Charge transfer in organic donor-acceptor systems from ultrafast non-adiabatic molecular dynamics simulation*
17:15	V. Heine Award Ceremony					
17:30						
17:45	COFFEE BREAK					
18:00	Mugaritz Restaurant, The Science of Cooking. Open to the General Public					
18:15						
18:30						
18:45						
19:00						
20:30	CONFERENCE GALA DINNER					

THURSDAY
SEPTEMBER 10, 2015

PLENARY TALK	SYMPOSIUM	INVITED TALK	CONTRIBUTED TALK

TIME	ROOM 6
09:00 to 12:00	Kurt Stokbro *Hands-on tutorial: Virtual NanoLab interface for atomic-scale modelling with ATK, FHI-aims, Quantum Espresso, VASP, LAMMPS, and others applications.*

TIME	AUDITORIUM (1.806)	CHAMBER HALL (624)	ROOMS 1+2+3 (575)	ROOM 10 (169)	ROOMS 4+5 (110)	ROOMS 8+9 (100)
09:00 09:15 09:30	Plenary 5 Jörg Neugebauer: *Mastering the structural and thermodynamic complexity of modern materials*		**S29 Electronic Structure Theory for Biophysics (cont'd).** Chairs: Leonardo Guidoni		**S28 Matter Under Extreme Conditions.** Chairs: Hardy Gross	
09:45	**S17 Topological Insulators.** Chairs: David Vanderbilt S17 I1 Irene Aguilera: *Importance of relativistic GW calculations for topological insulators*	**S5 Theoretical Spectroscopy.** Chairs: Zeilla Zanolli	S29 I3 Ursula Röthlisberger: *Origin of the Spectral Shifts among the Early Intermediates of the Rhodopsin Photocycle*	**S21 Hybrid Photovoltaic Materials.** Chairs: Wanda Andreoni	S28 I1 Dario Alfe: *Transport properties of iron mixtures at Earths core conditions*	**S26 Modeling of Defect Levels.** Chairs: Christoph Freysoldt
10:00		S5 I1 Peter Blaha: *Electron-hole interactions in theoretical spectroscopy*		S21 I1 Filippo de Angelis: *Modeling organohalide perovskites for photovoltaic applications: From materials to interfaces*		S26 I1 Audrius Alkauskas: *Radiative and nonradiative carrier capture at point defects: ab initio formulation of a classical problem*
10:15	S17 I2 Kevin Garrity: *First principles design of robust Chern insulators*		S29 C3 Jon Zubeltzu. *Structural and dynamical properties of nanoconfined liquid water and ice*		S28 I2 Yanming Ma: *Crystal Structure Prediction Boosting Up High Pressure Discoveries*	
10:30		S5 C1 Roberto Cardia. *Effects of substitution and functionalization on the electronic, optical, and transport properties of polycyclic aromatic hydrocarbons*	S29 C4 Daniele Varsano. *Protein field effects on electronic excitations of biological chromophores: a QMC and GW/BSE approach in QM/MM environment*	S21 C1 Carlo Motta. *Effects of the organic cation orientation in hybrid halide perovskites*		S26 I2 Hannu-Pekka Komsa: *Formation energies and defect levels of charged defects in 2D materials*
10:45	S17 C1 Yong Xu: *Recent Progresses on The Research of Two-Dimensional Stanene*	S5 I2 Jan Minar: *Theoretical description of angular momentum resolved photo emission on the basis of the one-step model - recent developments*	S29 I4 Daniele Bovi: *Ab-initio molecular dynamics studies of Photosystem II complex*	S21 C2 Menno Bokdam: *Optical absorption spectra and excitons of organometal halide perovskites*	S28 C1 Pasquale Pavone: *High-pressure and nonlinear elastic response of solids: Example of carbon allotropes*	

11:00	S17 I3 Junwei Liu: *Topological crystalline insulator: new physics and materials*			S21 I2 Andrew Rappe: *Shift Current and Ferroelectric Domain Walls in Organometal Halide Perovskites for Photovoltaic Applications*	S28 C2 Attila Cangi: *Improving Ab-Initio Methods for Warm Dense Matter Simulations*	S26 C1 Jun Cheng. *First principles determination of redox potentials from random phase approximation and double hybrid functional*
11:15		S5 I3 Patrick Rinke: *To GW and beyond: what we can learn from molecular calculations*	S29 I5 Johannes Neugebauer: *Density-Based Embedding for Chromophores in Proteins*		S28 I3 Kieron Burke: *DFT for warm dense matter*	S26 C2 Ferenc Tasnadi: *Vacancy formation energy in alloys: an example of TiAlN*
11:30	S17 C2 Hongming Weng: *Theoretical prediction of Topological semimetals*			S21 C3 Javad Hashemi. *Tuning the electronic and dielectric properties of solar cells: A strain-driven direct-to-indirect bandgap transition*		S26 I3 Sergey Levchenko: *Defect-defect interaction at surfaces and interfaces at realistic conditions: Global versus local effects of doping*
11:45	S17 C3 Domenico Di Sante. *Topological Tuning in Three Dimensional Dirac Semimetals*	S5 C2 Irina Lebedeva: *Time-dependent density functional theory of magneto-optical response of periodic insulators*	S29 C5 Joaquim Jornet-Somoza. *Untangling Excitonic Energy Transfer for the LHC-II complex from Full First-Principles Calculations*	S21 C4 Jarvist Moore Frost. *Hybrid halide perovskites: modelling crystal dynamics and devices*	S28 C3 Jonathan Lloyd-Williams: *Quantum Monte Carlo study of the phase diagram of solid molecular hydrogen at extreme pressures*	
12:00	S17 I4 Jürgen Henk: *Unexpected topological phases in topological insulators and in transition metals*	S5 I4 Maurits Haverkort *Ab initio methods for excitons, resonances and band excitations in time and frequency domain*	S29 C6 Elena Molteni. *A first-principle study of the atomic and electronic properties of thymine molecule adsorbed on the Silicon(001) surface*	S21 I3 Paolo Umari: *Modelling hybrid photovoltaic devices through accurate GW and BSE calculations*	S28 C4 Andreas Hermann: *New hydrogen bond network topologies in alkali hydroxides under pressure*	S26 C3 Yu Kumagai: *Electrostatics-based finite-size corrections for point defects in semiconductors*
12:15			S29 I6 Ville Kaila: *Multi-scale Molecular Simulations on Energy-Transducing Enzymes*		S28 I4 Ronald Redmer: *DFT applied to warm dense matter*	S26 C4 Al-Moatasem El-Sayed. *Hydrogen Induced Defect at Strained Si-O Bonds in Amorphous Silicon Dioxide*
12:30	S17 C4 Alexey Soluyanov: New type of Weyl semimetals with a material illustration	S5 C3 Umberto De Giovannini: *Modeling time and angle-resolved photoelectron spectroscopy with time-dependent density functional theory*		S21 I4 Feliciano Giustino: *Bridging the gap between theory and experiment in photovoltaic research*		S26 I4 Alfredo Pasquarello: *Determination of Defect Levels through Advanced Electronic Structure Methods*
12:45	S17 C5 Shu-Chun Wu: Topological surface states of the Heusler topological insulators	S5 C4 Ngoc-Linh Nguyen: *First-Principles Photoemission Spectroscopy in Molecules and Electronic Structure of Extended Systems from Koopmans-Compliant Functionals*	S29 C7 Eduardo Diaz Suarez. *Ab initio study of spectroscopic properties of porphyrins*			
13:00	Closing Session					
13:15						
13:30						