WORKSHOP mini 2012 on

COMPUTATIONAL CONDENSED MATTER PHYSICS, MATERIALS SCIENCE and NANOSCIENCE from FIRST PRINCIPLES

BARCELONA, **JANUARY 12-14** 2012

www.icmab.es/mini2012

SUMMARY

The workshop “Computational Condensed Matter Physics, Materials Science and Nanoscience from First-Principles” (mini2012) was held in Barcelona between the 12th and 14th of January 2012. This workshop was part of the series of “International Workshops on Computational Physics and Materials Science: Total Energy and Force Methods”, which take place at Trieste’s ICTP in odd years and at a different location in even years, the previous one having been in Shanghai in 2010. The workshop had around 90 participants, including invited speakers and members of the International Scientific Committee. We had very lively sessions covering the latest developments in first-principles methods, featuring quantum Monte Carlo techniques, new DFT functionals, and schemes for large scale simulations. The sessions focused on applications covered problems in magnetism and topological phases, electrochemistry and photocatalisys, electron dynamics, strong correlations, as well as miscellaneous topics in material science. The scientific quality of the talks and discussions was very high, and the same applies to the very crowded poster session that we had in the first evening. All in all, we believe the workshop succeeded in providing a broad view of the current state of the field, combined with some topics that are not so well-known to the community at large or to the regular attendees of the series. The activity was evaluated very positively by the International Scientific Committee and regular participants. This opinion is shared by the local organizers, as the workshop exceeded our expectations regarding both its scientific quality and the number and liveliness of the interactions it fostered.

SCIENTIFIC CONTENT AND DISCUSSIONS

The scientific content of the workshop revolved around the latest developments in first-principles electronic structure theory, and more generally on the application of cutting-edge numerical methods in nanoscience, condensed matter physics and materials science. The workshop was organized in a number of invited oral sessions, where internationally recognized experts were called to present what we judged to be the most significant advances of the past few years. While the specific topics of each session were diversified to offer a reliable snapshot of the current status of the field, there were some recurrent themes that characterized most of the oral presentations, namely: I) the reliable description of electron correlations, II) strategies to overcome the stringent time- and length-scale limitations of DFT, III) electron excitations, ultrafast dynamics and non-adiabatic processes; IV) magnetism and novel materials characterized by non-trivial band topologies. With the partial exception maybe of the last point (topological insulators are a class of materials where the most peculiar aspects of the physics can often be captured already at the single-particle level) these are the most outstanding and difficult challenges that the field is facing, and all the speakers did an excellent job at portraying the serious efforts that are being made worldwide, in order to make significant progress along these crucial methodological issues. Some of the sessions were more oriented towards applications, but nonetheless followed the traditional style of this series of conferences and workshops: dealing with systems or phenomena that are “difficult” to describe within standard density functional theory, and that require special care to cope, e.g. with quantum nuclear fluctuations in ice (M. Fernandez-Serra), or with the complexity of transition-metal oxides (J. Junquera, J. Kunes, T. Saha-Dasgupta). Most of the oral presentations generated lively discussions, demonstrating once more the novelty of the topics, which are not fully established within the community yet. Overall, we have the feeling that the theory sessions (e.g. on Quantum Monte Carlo, DFT Functionals, Electron Dynamics) were characterized by especially insightful debates, that we

believe have produced a constructive and fruitful exchange of ideas between the participants. Alongside the oral sessions, there was also a poster session where all participants were encouraged to present their results. At the end of the first day, after so many oral talks, we were pleasantly surprised to see that the participants weren't tired or intimidated by the sheer amount of information they were exposed to, and got involved into many discussions, thus contributing to a lively and successful poster session. In the poster session we were also pleased to see a large participation of young scientists working locally in Barcelona, and more generally in Spain. One of the motivations behind the “MINI” series of workshops is to give a marked priority to participants coming from the Country where the workshop is hosted. Also from this point of view, we can say that the workshop fulfilled our aims, and more generally the guidelines of the International Steering committee. All in all, the scientific contents of the workshop were in line with the tradition of high quality and attention to the cutting-edge developments that has characterized the “MINI” series throughout the years. At the same time, we succeeded at keeping a balance between formal theory and applications, so that the sessions could appeal to a broader audience. The encouragingly warm response, both from the scientific committee and by the regular participants, clearly confirmed this success.

RESULTS AND IMPACT FOR FUTURE DIRECTIONS OF THE FIELD

Given the extraordinarily high quality, diversity and interest of the presentations, it is impossible to discuss here the many ways in which this workshop may affect the scientific development of the field and the future work of their participants. Nevertheless, we believe some broadly-shared impressions can be highlighted.

- The quantum Monte Carlo (QMC) session was impressive for the quality of the methodological developments that were presented. Also, and maybe more interestingly, it reflected the momentous stage of the field, the current goal being to popularize QMC methods so that they become a mainstream tool inside the community, hence the proclaimed goal of producing QMC programs that can be used as a "black box". The situation for QMC was thus presented as comparable to that of DFT methods about 15 or 20 years ago; if this gets confirmed, it could change the way many difficult problems are treated in our community, as QMC could come as a very welcome tool for, at the very least, producing benchmark results to measure the accuracy of (or fit) other simpler approaches. At any rate, it is clear that QMC will be attracting renewed attention and efforts in coming years, and that many workers in the community will be paying a lot of attention to its evolution.

- Another approach that attracted great interest was density matrix functional theory (DMFT), especially in what regards its application to magnetic systems. This issue led to very lively discussions during the workshop and, at a minimum, the conclusions are that (1) there is an urgent need to develop DMFT in this area and (2) there is a language breach that needs to be closed between DMFT experts and workers on applications of first-principles methods to magnetic problems (e.g., to strongly-correlated-electron systems). We think the workshop was very effective in

evidencing these issues and motivating the community to take action about them in the near future.

- The new methods for accurate time-dependent density functional theory (TDDFT) simulations of solids were an eye-opener for many participants of the workshop. The presentations on the topic received great interest, and the urgent need to further develop and popularize such methodologies was made clear. Again, we think the workshop was very effective in bringing together the developers of new methods and the (large) community of potential users, which we think guarantees effective and increased activity along these lines in the future.

- Finally, the short but intense session on large scale simulations featured various elegant and suggestive approaches for both hybrid (system-embedding based) and full *ab initio* simulations of very big systems. The spectacular results presented by both speakers (J. Neugebauer and J. VandeVondele) constituted strong motivation for other code developers to implement/improve the new schemes, which should lead to their desirable generalization and application to a variety of (probably more challenging) problems. Here again, we think our workshop served its purpose and will contribute to shape much future activity in the field.

ANNEXES

Scientific Program

Thursday, January 12th, 2012

Morning

08:30 REGISTRATION

08:50 OPENING REMARKS

09:00-11:00 SESSION: **Quantum Monte Carlo** - Chair: Claudia Filippi (U. Twente)

09:00 **Ali Alavi** (University of Cambridge, UK)
Quantum Monte Carlo approach to the full CI problem: recent progress

09:40 **Sandro Sorella** (SISSA, Italy)
Efficient Resonance Valence Bond approach for electronic structure

10:20 **Shiwei Zhang** (College of William and Mary, USA)
Recent progress in electronic structure calculations by auxiliary-field quantum Monte Carlo

11:00-11:30 COFFEE BREAK

11:30-12:50 SESSION: **Materials I** - Chair: Nicola Marzari (EPFL)

11:30 **Mariví Fernandez-Serra** (Stony Brook University, USA)
Anomalous Nuclear Quantum Effects in Ice

12:10 **Javier Junquera** (Universidad de Cantabria, Spain)
Highly-confined spin-polarized two-dimensional electron gas in $SrTiO_3/SrRuO_3$

13:00-15:00 LUNCH BREAK

Afternoon

15:00-17:00 SESSION: **Magnetism and Topological Phases** - Chair: David Vanderbilt (Rutgers)

15:00 **Stefan Blügel** (Jülich Forschungszentrum, Germany)
Spin relaxation mechanisms in metallic systems: Resonance and anisotropy effects

15:40 **Ivo Souza** (Universidad del País Vasco, Spain)
Wannier-based description of orbital magnetic effects in ferromagnets

16:20 **Oleg Yazyev** (EPFL, Switzerland)
Bismuth chalcogenide topological insulators from first principles

17:00-19:00 COFFEE BREAK & POSTER SESSION

Friday, January 13th, 2012

Morning

09:00-11:00 SESSION: **New DFT Functionals** - Chair: Lucia Reining (École Polytechnique)

09:00 **Sangeeta Sharma** (Max Planck Halle, Germany)
Treatment of strongly correlated systems within the framework of reduced density matrix functional theory

09:40 **Gustavo E. Scuseria** (Rice University, USA)
Symmetry breaking and restoration in electronic structure theory

10:20 **Andreas Savin** (Université Pierre et Marie Curie, France)
Coupling wave function with density functional calculations

11:00-11:30 COFFEE BREAK

11:30-12:50 SESSION: **Electrochem. & Photocatalysis** - Chair: Shobhana Narasimhan (JNCASR)

11:30 **Annabella Selloni** (Princeton University, USA)
First principles simulations of materials and processes in photo- and electro-catalysis

12:10 **Michiel Sprik** (University of Cambridge, UK)
Reactivity of holes at the TiO2/water interface

13:00-15:00 LUNCH BREAK

Afternoon

15:00-17:00 SESSION: **Electron Dynamics** - Chair: Steven G. Louie (UC Berkeley)

15:00 **Matteo Gatti** (Universidad del País Vasco, Spain)
Design of effective kernels for spectroscopy: time-dependent current-density-functional theory

15:40 **Fernando Martín** (Universidad Autónoma de Madrid, Spain)
XUV/X-ray femto- and attosecond laser pulses for ultrafast electronic control in simple molecules: towards attochemistry?

16:20 **Marco Schirò** (Princeton University, USA)
Dynamics of Strongly Correlated Electrons out of Equilibrium

17:00-17:30 COFFEE BREAK

17:30-18:50 SESSION: **Large Scale Simulations** - Chair: Richard M. Martin (U. of Illinois)

17:30 **Johannes Neugebauer** (TU Braunschweig, Germany)
Subsystem-Based Time-Dependent Density-Functional Theory for Biomolecular Spectroscopy

18:10 **Joost VandeVondele** (University of Zürich, Switzerland)
Simulating large condensed phase systems with GGA and hybrid density functionals

Evening

20:30 CONFERENCE DINNER

Saturday, January 14th, 2012

Morning

09:00-11:00 SESSION: **Materials II** - Chair: Xingao Gong (Fudan U.)

09:00 **Jörg Neugebauer** (Max Planck Düsseldorf, Germany)
Fully ab initio determination of free energies: Application to modern high-strength steels

09:40 **Cheol-Hwan Park** (Massachusetts Institute of Technology, USA)
Many-body effects on the carrier dynamics of graphene

10:20 **Rubén Pérez** (Universidad Autónoma de Madrid, Spain)
Probing nanostructures with forces and currents

11:00-11:30 COFFEE BREAK

11:30-12:50 SESSION: **Strong Correlations** - Chair: Eric Koch (Jülich)

11:30 **Jan Kuneš** (Academy of Sciences, Czech Republic)
Thermal and doping effects in materials with competing multiplets

12:10 **Tanusri Saha Dasgupta** (SN Bose Centre for Basic Sciences, India)
A Realistic Theory of Correlated Oxides

12:50 CLOSING REMARKS

13:00-15:00 LUNCH

Invited Speakers

Andreas Savin, Universite Pierre et Marie Curie, France
Gustavo E. Scuseria, Rice University, USA
Sangeeta Sharma, Max Planck Halle, Germany
Ali Alavi, University of Cambridge, UK
Sandro Sorella, SISSA, Italy
Shiwei Zhang, College of William and Mary, USA
Stefan Blügel, Jülich Forschungszentrum, Germany
Ivo Souza, Universidad del País Vasco, Spain
Oleg Yazyev, EPFL, Switzerland
Jan Kunes, Academy of Sciences, Czech Republic
Tanusri Saha Dasgupta, SN Bose National Centre for Basic Sciences, India
Matteo Gatti, Universidad del Pais Vasco, Spain
Fernando Martin, Universidad Autonoma de Madrid, Spain
Marco Schiro, Princeton University, USA
Annabella Selloni, Princeton University, USA
Michiel Sprik, University of Cambridge, UK
Marivi Fernandez-Serra, Stony Brook University, USA
Javier Junquera, Universidad de Cantabria, Spain
Jorg Neugebauer, Max Planck Dusseldorf, Germany
Cheol Hwan Park, Massachusetts Institute of Technology, USA
Ruben Perez, Universidad Autonoma de Madrid, Spain
Johaness Neugebauer, Technical University Braunschweig, Germany
Joost VandeVondele, University of Zurich, Switzerland

PARTICIPANTS

Sientific Committee (attending the workshop)

Stefano Baroni, SISSA - Trieste, Italy
Claudia Filippi, Univ. Twente, Netherlands
Xingao Gong, Fudan University, China
Francesco Mauri, Univ. Pierre et Marie Curie,France
Erik Koch, Forschungszentrum Jülich, Germany
Steven G. Louie, Univ. California - Berkeley, USA
Richard M. Martin, University of Illinois, USA
Nicola Marzari, EPFL, Switzerland
Shobhana Narasimhan, JNCASR - Bangalore, India
Lucia Reining, École Polytechnique - Paris, France
David Vanderbilt, Rutgers University, USA

Organizing Committee (attending the workshop)

Pablo Ordejón, CIN2, Spain
Jorge Iñiguez, ICMAB, Spain
Massimilano Stengel, ICMAB, Spain
Daniel Sanchez-Portal, Centro de Física de Materiales, Spain

Other participants

Hideaki Sawada, Nippon Steel Corporation, JAPAN
Josep María Oliva, Instituto Rocasolano - CSIC, Spain
Alberto Marmodoro, Max-Planck-Institut für Mikrostrukturphysik, Germany
Jose María Soler,Universidad Autónoma de Madrid, Spain
Peter Koval, Centro de Fisica de Materiales - Donostia, Spain
Nicolai A. Bogdanov, Inst. Theoretical Solid State Physics - Dresden, Germany
David Soriano, ICN, Spain
P. Andre Clayborne, University of Jyväskylä, Finland
Perla Wahnón, UPM, Spain
Diego Carrascal, Univ. Oviedo, Spain
Gian-Giacomo Asara, U. Rovira i Virgili, Spain
Christina Ebensperger, University Erlangen-Nürnberg, Germany
Michelle Fritz, U. Autonoma de Madrid, Spain
Julen Ibañez, Donostia Int. Physics Center, Spain
Jon Mikel Azpiroz, UPV/EHU, Spain
Elisa Jimenez, UPV/EHU, Spain
Andres Vega, Universidad De Valladolid, Spain
Lauro O. Paz Borbon, C. C. Catalysis - Chalmers, Sweden

Emilio Artacho, Nanogune, Spain
Yohanna Seminovki, UPM, Spain
Federico Iori, Universita Di Modena, Italy
Silvia Gallego, CSIC, Spain
Jae Kyung Chang, Sugkyunkwan University, Korea
Changhyun Yi, Sugkyunkwan University, Korea
Kjartan Thor Wikfeldt, University College London, UK
Nadia Binggeli, ICTP, Italy
Ju-Yong Kim, Sugkyunkwan University, Korea
Guillermo Roman-Perez, UAM, Spain
Kerstin Hummer, University Of Vienna, Austria
Gabriel Bester, Max Planck Inst., Germany
Idoia G.De Gurtubay, UPV/EHU, Spain
Jose Javier Plata, Universidad De Sevilla, Spain
Alberto García, ICMAB, Spain
Otto González, ICMAB, Spain
Mathias Ljungberg, ICMAB, Spain
Claudio Cazorla,ICMAB, Spain
Desanka Boskovic, CIN2, Spain
Jose Angel Silva, CIN2, Spain
Rafael Martínez, CIN2, Spain
Jacek Wojdel, ICMAB, Spain
Oswaldo Dieguez, ICMAB, Spain
Ricardo Rurali, ICMAB Spain
Alvaro, Miranda, ICMAB, Spain
Miguel Pruneda, CIN2, Spain
Carlos F. Sanz-Navarro,CIN2, Spain
Oscar Paz, ICMAB, Spain