Science Meeting – Scientific Report

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ESF Science Meeting
Reference Number: 5760
ESF Activity
Unit(s): PESC
Activity Title: Advanced Concepts in Ab Initio Simulations of Materials
Activity Acronym: Psi-K2
PROJECT
Science Meeting: Workshop
Title of Science Meeting: Computer Simulations of Condensed Phase Systems - From Correlated Electrons to Novel Materials
Location: CNR Headquarters, Piazzale Aldo Moro 7, Rome (Italy)
Date of Science Meeting: 4/5/2015 – 6/5/2015
Convenors' Names: Dr Fabio Affinito (CINECA, Bologna, Italy), Dr Paola Alippi (CNR ISM, Rome, Italy), Dr Claudio Attaccalite (CNRS, Grenoble, France), Dr Lilia Boeri (TU Graz, Austria), Dr Michele Cascella (University of Oslo, Norway), Dr Paola Gori-Giorgi (VU University Amsterdam, The Netherlands), Dr Leonardo Guidoni (University of L'Aquila, Italy), Dr Daniele Varsano (CNR Nano, Modena, Italy)

SUMMARY (up to 1 page)

The workshop "Computer simulations for condensed phase systems: from correlated electrons to novel materials" took place in Rome, at the headquarters of the CNR (Italian National Research Council) , on the 4th and 5th of May 2015. It was meant as a celebration of Giovanni Bachelet's 60th birthday, organized by several of his former students who are currently active in the field of electronic structure calculations.

Giovanni Bachelet has been one of the pioneers in the field. After graduating with F. Bassani, he moved to the Bell Labs (USA), where he made key contributions to pseudopotentials theory and practice; he was then active in several European institutions (MPI Stuttgart, Scuola Normale di Pisa, CNR Trento), before being appointed a professorship in condensed matter theory at the University la Sapienza, Rome, where he is still today. Beside his activity on a wide range of topics over the years (especially on methodological developments such as pseudopotentials, beyond-local density functionals, and Quantum Monte Carlo), Giovanni has been an important actor in the electronic structure community also through his mentoring, organizational and teaching activity; many of his former students and collaborators are now established independent researchers at several European institutions.

The scope of this workshop was to bring together many colleagues and collaborators of Giovanni from different stages of his career at his own research institution. This automatically provides for a remarkable roster of speakers, who are all leading experts in the different areas of electronic structure theory which have taken the stage over the years (Density Functional Theory, electronic structure of real materials, correlated electrons, molecular dynamics, quantum Monte Carlo, theoretical spectroscopy). The workshop mapped out the progress of ab initio electronic structure theory over the last 30+ years through the very voices of many of its leading figures, touching upon key developments, from electron-electron interaction via functionals or Monte Carlo through to cutting edge applications to nanoscience.

The format of the workshop has been carefully designed to encourage exchange and discussion between participants at all levels. The scientific program comprised two scientific sessions with 20 invited speakers, a “round-table” moderated by Giovanni Bachelet, where some of his former students briefly presented their most recent results and a poster session. The event was advertised using several channels and we had a participation of more than 70 people among researchers and students.

2. Description of the scientific content of and discussions at the event (up to four pages)

In this section we describe the scientific content and discussions in the three days of the conference.

Day 1:
The opening session was introduced by the chairman of the CNR, **Luigi Nicolais**, who recalled the importance of the role of Giovanni Bachelet both as a scientist and as a politician for the development of the italian scientific community. Then **Angelo Vulpiani** talked about a statistical mechanics approach to the chaos theory using the case of condensed matter theory as an example for reductionism. The following talk was given by **Federico Capasso**, who spoke about an example of applied physics. He showed what metasurfaces are and their use for the design of optical components.

The second session of the first day started with a multidisciplinary seminar from **Luciano Pietronero** who illustrated an example of how statistical physics can be successfully used in economics. To evaluate the "economical fitness" of different countries he has introduced a model which is able to catch the differences between different regimes, and, at the same, it can suggests which are the future economic trends of the countries. The second and third talks were on the subject of ab initio molecular dynamics for research in sustainable development, a field in rapid expansion in the recent years. Monoethanolamine solutions are commonly used for the sequestration of carbon dioxide from the atmosphere, but the exact chemical mechanisms underlying this process are still unclear. Using ab initio molecular dynamics simulations **Wanda Andreoni** better characterised the chemical reactions occurring during this process, suggesting which chemical steps are occurring during the carbon dioxide dissolution. The talk of **Annabella Selloni** was on the catalytic mechanisms of transition metal oxides for water splitting, a reaction which has an important role for the future possibilities to obtain clean energy from sunlight. In particular, she has shown some recent result on the mechanisms of water splitting on titania-water surfaces, illustrating the role of proton-coupled-electron-transfer in this reaction. **Michele Parrinello** has illustrated the basic concepts of metadynamics and some recent applications. Metadynamics was used to investigate the nucleation phenomenon of crystals formation starting from solution. These simulations allow to understand the mechanisms of crystal growth and, at the same time, to estimate nucleation rates.
The afternoon session included four talks spanning different topics related to structure and properties of solid state materials. The first talk by Prof. **O.K. Andersen** discussed the band structure of purple bronze $LiMo_6O_{17}$ and the origin of its one-dimensional behaviour. The second talk by Prof. **D. Hamann** focused instead on development of pseudo-potentials, from the original Bachelet-Hamann-Schlueter table to most recent ONCVPSP norm-conserving formalism. Prof. **S. Louie** presented theoretical studies on quasi-2D systems (mono- or few-layered dichalcogenides and graphene). The presented calculations evidence the possibility of appearance of several quantum phenomena in such systems, like exciton separation or tunable magnetism. The last talk of the session was given by Prof. **R. Car**, who exposed recent development in inclusion of dispersion forces within a DFT formalism, and its applicability for studies of van-der-Waals dominated molecular crystals.

Day 2:
The second morning session was mainly devoted to recent advances in Quantum Monte Carlo (QMC) methods. In the first talk, Prof. **C. J. Umrigar** gave a comprehensive overview of different stochastic approaches to the many-body Schroedinger equation, both in the continuum and in determinantal space, illustrating the advantages and disadvantages of different projectors. He then illustrated his recent results on a mixed scheme (combining exact diagonalization and stochastic sampling), which largely improves the full-CI QMC method of Alavi and coworkers. Right after him, Prof. **S. Fahy** presented his work on first-principle calculations (DFT based) of ultrafast photoexcitation and decay of coherent phonons in photo-excited bismuth, discussing different aspects, and providing an extensive overview on the available experimental data.

Prof. **S. Sorella**, then discussed his auxiliary field QMC results on phase separation in the two-dimensional (2D) Hubbard model. Using a new technique that drastically reduces size effects in the extrapolation to the thermodynamic limit, he could finally address an important question (on which several different claims have been done in the past years), showing that, indeed, there is phase separation in the 2D Hubbard model for specific ranges of parameter values. Finally, dr. **S. Moroni** presented a QMC study of the superfluid-crystal quantum phase transition of a system of purely repulsive dipolar bosons in two dimensions. He showed that the microemulsion scenario for any physical realization of this system is ruled out, given the exceedingly large predicted size of the bubbles.

Day 3:
In the third day there were been three important talks on different aspect of the scientific research. In the first talk professor **G. Jacucci** discussed how the outcome of the phenomenological observation may depend from the observer. This fact has important implication in the development science and scientific knowledge. In the second talk professor **M. Altarelli** made a comprehensive introduction to the potentiality of the new free electron lasers. In particular he focused on the possibility to resolve atomic structure of cluster, proteins and other materials without the need of crystallizations. Then he presented some preliminary work on the study of correlation functions in liquids and other systems. Finally in the last professor **E. Tosatti** discussed the dichotomy between models and ab-initio calculations. He showed, with some remarkable examples, that the combination of these two approaches can bring to a better understanding and interpretation of new physical phenomena.

3) Assessment of the results and impact of the event on the future directions of the field (up to two pages)

This workshop, with participants coming from across the world, is a good example of international collaboration. The presence of a large spectra of subjects and different approaches used to solve complicated problems in condensed matter physics opened the possibility to new and unexpected collaborations among the participants. The discussions that followed each presentation demonstrated the interest of the participants in research areas sometime different from their own ones.
The main outcome of the workshop is the need of combining different approaches to get a better understanding and interpretation of new physical phenomena at different scales.
We think that the format of the present workshop can facilitate this kind of collaborations and we hope in the future to organize more often similar conferences.

ABSTRACTS OF THE LECTURES
see PDF in attachment

Annexes 4a) and 4b): Programme of the meeting
see PDF in attachment

full list of speakers and participants

LIST OF PARTICIPANTS

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Guido Chiarotti
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FINAL PROGRAMME

Day 1

8:30 Registration

9:00 Paola Alippi: Welcome
9:30 Luigi Nicolais: Introduction
10:00 Angelo Vulpiani: A (random) tour around quantum mechanics, condensed matter and reductionism
10:30 Federico Capasso: Structured light with metasurfaces

11:00 Coffee break

11:30 Luciano Pietronero: New metrics for economic complexity: the intangible fitness of countries and complexity of products
12:00 Wanda Andreoni: CO_2 capture in amine solutions: an update on modeling and simulations
12:30 Annabella Selloni: Water adsorption and oxidation on metal oxides
13:00 Michele Parrinello: Atomistic modeling of crystal nucleation and growth

13:30 Lunch Break

15:00 Ole K. Andersen: Band structure of the purple bronze $LiMo_6O_{17}$
15:30 Donald R. Hamann: Ab initio pseudopotentials: from BHS to ONCVPSP
16:00 Steven G. Louie: Electrons and excitons in quasi 2D materials
16:30 Roberto Car: van der Waals bonded crystals: a challenge for density functional theory

17:00 Coffee break

17:30 Poster session

20:30 Social Dinner

Day 2

9:00 Annalisa Fasolino: Subbands and new oxygen heterostructures: the LaAlO3/SrTiO3 interface
9:30 Elisa Molinari: Exciting graphene nanostructures
10:00 Matthias Scheffler: Big data of materials science - critical role of the descriptor

10:30 Stefano Baroni: What I cannot compute I do not understand: fathoming atomic heat transport from the struggle to simulate it!

11:00 Coffee break

11:30 Cyrus J. Umrigar: Zero temperature quantum Monte Carlo methods and the sign problem
12:00 Stephen Fahy: Ultrafast photoexcitation and decay of coherent phonons
12:30 Sandro Sorella: What about phase separation in the Hubbard model?
13:00 Saverio Moroni: Coexistence, interfacial energy and microemulsions in 2D dipolar bosons.

13:30 Lunch break

15:00 Discussion: Who cares about cores?

17:00 Coffee break

17:30 Poster session

Day 3

9:00 Gianni Jacucci: Autopoiesis and cognition, an outstanding outcome of phenomenology
9:30 Massimo Altarelli: Theory challenges from X-ray free-electron lasers
10:00 Erio Tosatti: Modeling versus realistic first-principles calculations/ simulations in condensed matter theory
10:30 Michele Cascella: Closing remarks

See separate pages below
FINANCIAL REPORT

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