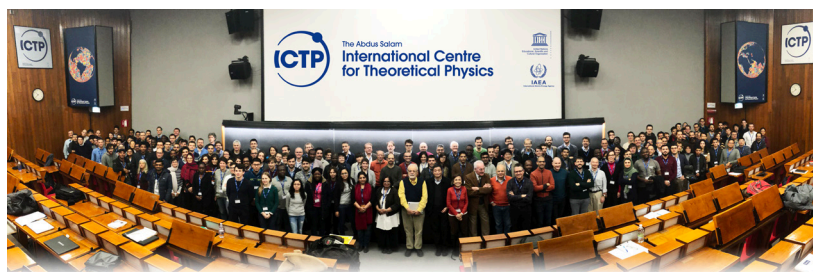


SCIENTIFIC REPORT ON THE 19TH INTERNATIONAL WORKSHOP ON COMPUTATIONAL PHYSICS AND MATERIAL SCIENCE: Total Energy and Force Methods

Abdus Salam International Centre for Theoretical Physics, Trieste (Italy)
09 Jan 2019-11 Jan 2019



19th International Workshop on
Computational Physics and Material Science: Total Energy and Force Methods

9 - 11 January 2019, Miramare - Trieste, Italy

Group photo of the Workshop on “19TH INTERNATIONAL WORKSHOP ON COMPUTATIONAL PHYSICS AND MATERIAL SCIENCE: Total Energy and Force Methods, 09 Jan 2019-11 Jan 2019

The “Total Energy” Workshop has been held traditionally in Trieste every two years since 1987. This year, the Workshop is about recent progress in electronic structure methods and their applications. The aim is a critical discussion of methods and of possible combinations and challenging applications. It has become one of the most popular regular events of the international ab-initio electronic structure community. This event also has the ambition to reach out to countries where the electronic structure community is not traditionally as strong as in Europe, the USA and Japan, in coherence with the missions of its traditional host institution, the ICTP.

This event took place at the ICTP Leonardo Building in the Budinich Hall. The format included 24 (long) oral presentations given by invited speakers and a total of 110 poster presentations. The workshop was attended by a total of 240 participants (including directors and speakers) from 27 countries.

Organizers:

Jeffrey Neaton (University of California, Berkeley, USA)

Mike Finnis (Imperial College, London, UK)

Marilia Caldas (University of Sao Paulo, Brazil)

Local Organizers:

Ali Hassanali (The Abdus Salam International Centre for Theoretical Physics)

This event has been sponsored by ICTP, SISSA and the Psi-k Network.

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The Workshop focuses on recent progress in electronic structure methods and their applications to a steadily increasing range of materials and systems. The most widespread approaches used in our community are DFT, TDDFT, GW, DMFT, and quantum Monte Carlo methods, which provide the foundation for computing many physical and chemical properties of solids, liquids, and low-

dimensional systems. There are numerous challenging applications for which the levels of approximation used in these implementations, or their technical limitations, do not yet permit accurate quantitative predictions of some properties of materials. The goal of the Workshop is to give an in-depth analysis of a selection of scientific cases and applications. Cutting edge topics such as the use of multiscale modeling and machine learning will also form part of the programme.

Scientific Topics Covered:

- Quantum Materials: Topology and Correlation;
- Strong Correlations in Quantum Chemistry;
- Excited-State Phenomena: New Approaches and Applications;
- 2D Materials and Heterostructures;
- Dynamics at Complex Interfaces;
- Advances in Molecular Dynamics for Bridging Scales;
- Machine Learning for Methods and Applications.

Besides the scientific program of talks documented below, the conference included three other scientific programs that were integrated into the Total Energy workshop and made the activity rather unique:

1. Award of the Walter-Kohn Prize. The Walter Kohn Prize for quantum-mechanical materials modeling, jointly instituted and co-funded by ICTP and the Quantum ESPRESSO Foundation is awarded biennially to a young scientist for outstanding contributions in the field of quantum-mechanical materials and molecular modeling, performed in a developing country or emerging economy, with emphasis on first-principles techniques. The Prize is usually awarded to one person, but may be shared equally among recipients who have contributed to the same body of work. The 2018 prize was given to Gabriel Merino, a researcher from Centro de Investigación y de Estudios Avanzados (Cinvestav), Unidad Mérida, Mexico. The prize recognizes his pioneering work on predicting and understanding novel systems that violate standard chemical paradigms, and for generalizing and broadening the scope of concepts such as aromaticity, coordination and the chemical bond.
2. The ICTP Prize was created in 1982 by the ICTP Scientific Council to recognize outstanding and original contributions in physics by young scientists (those who have obtained their PhD less than 12 years earlier) from, and working in, developing countries. The ICTP Prize includes a sculpture, certificate and a cash award of Euro 3000. ICTP has awarded its 2018 ICTP Prize to Luis E.F. Foà Torres of the University of Chile, Santiago, Chile, and to Hongjun Xiang of Fudan University, Shanghai, China. The Prize recognizes their independent contributions to the theoretical advancement of condensed matter physics of modern solid-state materials, including low dimensional and nanoscale systems. Theory work by Luis Foà Torres contributed importantly to our understanding of topological insulators, graphene and two-dimensional materials and nanotubes, including quantum transport and optoelectronics. Hongjun Xiang developed first-principles-based computational methods addressing a vast variety of problems, including low-dimensional materials and multiferroics, where his approach has become standard in the field. The groups of Foà Torres in Chile and Xiang in China constitute local centres of excellence whose research and collaboration activities launch students and postdocs into the widest international context.
3. The Total Energy Workshop also included a session dedicated as a tribute to Prof. Alessandro de Vita who tragically passed away last year. This session included short presentations on both the scientific and human contributions of Alessandro who was a regular attendee of the workshop in the past and made very important contributions in the field of computation.

4. Finally, in the spirit of the Walter Kohn prize that was awarded, we also had a session on electronic structure in Africa where the director of one of our new partner institutes, The East African Institute of Fundamental Research (EAIFR), Omololu Akin-Ojo, gave a talk about the computational sciences in Africa.

Below you will find a list of the invited talks in the Total Energy 2019:

LIST OF INVITED TALKS

AKIN-OJO, Omololu (ICTP East African Institute of Fundamental Research (EAIFR), University Rwanda, Kigali)

[Total energy and forces in Africa](#)

BIERMANN, Silke (Ecole Polytechnique, Palaiseau, France)

[Non-local interactions and non-local correlations: examples of dynamical mean field calculations for realistic materials](#)

CERIOTTI, Michele (EPFL, Switzerland)

[Physics-based machine learning for atomistic modelling](#)

COCCHI, Caterina (Humboldt Universitaet zu Berlin, Germany)

[Optical and core spectroscopy from many-body perturbation theory](#)

CSANYI, Gabor (University of Cambridge, U.K.)

[Interatomic potentials from first principles](#)

EDER, Robert (Karlsruhe Institute of Technology, Wuerttemberg, Germany)

[Electronic structure of transition metal compounds by variational cluster approximation](#)

FOA TORRES, Luis E.F. (Universidad de Chile, Santiago)

[Using Light as a Topological Switch](#)

KUNES, Jan (Vienna University of Technology, Austria)

[Dynamical susceptibilities and spontaneous symmetry breaking with dynamical mean-field theory](#)

MARZARI, Nicola (Ecole Polytechnique Federal de Lausanne, Switzerland)

[Computational materials discovery: good data vs big data](#)

MERINO, Gabriel (CINVESTAV, Unidad Merida, Mexico)

[Walter Kohn Prize Ceremony and Lecture](#)

MIRANDA RODRIGUES, Caetano (Universdade de Sao Paulo, Brazil)

[A sounded journey from nano to macro into everyday materials through multiscale molecular simulations](#)

MONSERRAT SANCHEZ, Bartomeu (University of Cambridge, U.K.)

[Optoelectronic properties at finite temperature](#)

NARASIMHAN, Shobhana (Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India)

[Descriptors from small data: Simple yet successful descriptors for self-assembly of organic molecules on surfaces](#)

NEESE, Frank (Max Planck Institut fuer Kohlenforschung, Muelheim an der Ruhr, Germany)

[Application of accurate wavefunction based methods to solids and surfaces](#)

PAVARINI, Eva (Forschungszentrum Juelich, Germany)

[Understanding strong-correlation effects in spin-orbit t2g materials](#)

PIGNEDOLI, Carlo A. (EMPA, Duebendorf, Switzerland)

[On-surface synthesis of graphene nanoribbons from computational perspective](#)

QUEK, Su Ying (National University of Singapore)

[Electronic screening of quasiparticle excitations by atomically thin substrates](#)

SOLUYANOV, Alexey (University of Zurich, Switzerland)

[Standard model for crystalline materials: beyond the elementary particles and the 10-fold classification of non-interacting topological phases](#)

TODOROVA, Mira (Max-Planck-Institut fuer Eisenforschung, Dusseldorf, Germany)

[Modelling electrochemical solid/liquid interfaces by first principles calculations](#)

VAN DE WALLE, Christian (University of California @ Santa Barbara, U.S.A.)

[Modelling point defects for quantum information science](#)

VANDERBILT, David H. (Rutgers, The State University of New Jersey, Piscataway, U.S.A.)

[Axion coupling in magnetoelectric and topological materials](#)

WEBER, Cedric (King's College London, U.K.)

[Many body effects in transition metal oxygen transport with dynamical mean-field theory](#)

WILHELM, Jan (BASF SE, Ludwigshafen, Germany)

[Low-scaling GW calculations using Gaussian basis functions](#)

XIANG, Hongjun (Fudan University, Shanghai, China)

[Theoretical Studies on New Mechanisms of Ferroelectricity and Multiferroicity](#)

Full details of the program can be found online at the following website:

<http://indico.ictp.it/event/8658/>