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

ICTP

9 - 11 January 2019
Trieste, Italy

Further information:
http://indico.ictp.it/event/8658/
smr3266@ictp.it

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.

Description:

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.

Topics:

- 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.

Scientific Advisory Committee:

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M. CALDAS, USP, Brazil
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J. B. NEATON, University of California, Berkeley, U.S.A.

Local Organizer:

A. HASSANALI, ICTP, Trieste, Italy

Speakers:

S. Biermann, Ecole Polytechnique, CNRS
A. Botana, Arizona State University
K. Burke, University of California, Irvine
M. Ceriotti, EPFL
C. Cocchi, Humboldt University, Berlin
G. Csanyi, University of Cambridge
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D. Vanderbilt, Rutgers University
C. Weber, King's College London
J. Wilhelm, BASF
H. Xiang, Fudan University

How to apply:

Online application:
http://indico.ictp.it/event/8658/

Female scientists are encouraged to apply.

Grants:

A limited number of grants are available to support the attendance of selected participants, with priority given to participants from developing countries. There is no registration fee.

Deadline:

15 October 2018

ICTP
The Abdus Salam
International Centre for Theoretical Physics
www.ictp.it
Trieste, Italy