



The Abdus Salam  
International Centre  
for Theoretical Physics



# 22nd International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods

## Description:

The “Total Energy” is a renowned workshop about recent progress in electronic structure methods and their applications. It has been held traditionally in Trieste every two years since the 1980s and has become one of the most popular regular events of the international *ab initio* electronic structure community.

## MORE DETAILS:

The goal of the workshop is to provide a broad view of recent developments, current challenges, and future directions of the field.

The program features invited talks and focused sessions on:

- novel energy functionals
- machine learning: theory and applications
- correlated materials and excited states
- electron-phonon coupling
- materials design and discovery
- quantum computing: applications and materials platforms
- time-dependent and out-of-equilibrium phenomena
- electronic structure grand challenges in the age of AI and quantum computing (discussion session)
- semiconductors and ferroelectrics (in memory of Alfonso Baldereschi)

The workshop will also include the award ceremony for the “Walter Kohn Prize for quantum mechanical material modeling” <https://www.ictp.it/about-ictp/prizes-awards/walter-kohn-prize.aspx>, co-funded by ICTP and the Quantum ESPRESSO Foundation.

## INVITED SPEAKERS:

Federica Agostini  
University Paris-Saclay, France  
Emilio Martin Artacho Cortés  
CIC nanoGUNE, Spain  
Raffaello Bianco  
University of Modena and Reggio Emilia, Italy  
Giovanni Caldarelli  
University of Rome “La Sapienza”, Italy  
Roberto Car  
Princeton University, USA  
Giuseppe Carleo  
EPFL, Switzerland  
Gábor Csányi  
University of Cambridge, UK  
Maria Chatzieftheriou  
Goethe University Frankfurt, Germany  
Nicola Colonna  
Paul Scherrer Institute, Switzerland  
Tommaso Chiarotti  
Caltech, USA  
Giulia Galli  
University of Chicago, USA  
Vikram Gavini  
University of Michigan, USA

Emmanouil Kioupakis  
University of Michigan, USA  
Leeor Kronik  
Weizman Institute, Israel  
Roxane Margine  
Binghamton University, USA  
Nisanth Nair  
IIT Kanpur, India  
Mariana Rossi  
Max Planck Hamburg, Germany  
Maria Clelia Righi  
University of Bologna, Italy,  
Gianluca Stefanucci  
University of Rome Tor Vergata, Italy  
Massimiliano Stengel  
ICREA, Spain  
Andrea Urru  
Rutgers University, USA  
QuanSheng Wu  
Institute of Physics, Chinese Academy of Sciences, China  
Claudio Zeni  
Microsoft Research AI4Science, UK

A limited number of contributed abstracts will be selected for upgrade to invited presentations.



8 - 10 January 2025



Trieste, Italy



Deadline:  
14 November 2024

## DIRECTORS:

Ion Errea, UPV/EHU, Spain  
Antimo Marrazzo, SISSA, Italy  
Shobhana Narasimhan, Jawaharlal Nehru Centre for Advanced Scientific Research, India  
Gian-Marco Rignanese, University of Louvain, Belgium

## LOCAL ORGANISER:

Ralph Gebauer, ICTP, Italy

## FURTHER INFORMATION:

E-mail: [smr4050@ictp.it](mailto:smr4050@ictp.it)

Web: <http://indico.ictp.it/event/10815/>

Junior and female scientists are particularly encouraged to apply



## REGISTRATION:

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.

