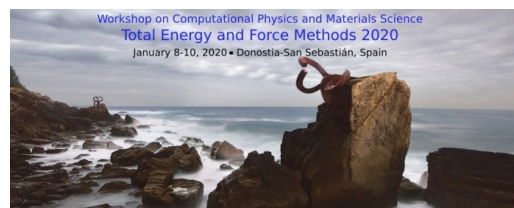




Workshop on Computational Physics and Materials Science: Total Energy and Force Methods (MiniTotalEnergy2 020)



08.Jan - 10.Jan 2020

Cod. Z01-20

Mod.:

Face-to-face

Edition

2020

Activity type

Workshop

Date

08.Jan - 10.Jan 2020

Location

Carlos Santamaría Zentroa

Languages

English

Academic Validity

30 hours

Organising Committee

Fundación
BBVA



Description

This workshop is organized within the “Total Energy and Force” conference series, which is held at ICTP in Trieste every odd year, and at a different place every even year. The previous most recent workshops of this “mini” series took place in Barcelona (2012), Lausanne (2014), Luxembourg (2016) and Cambridge (2018).

The core areas for the workshop series have traditionally been:

- Theory and methods: Density-functional theory beyond LDA, time-dependent DFT, manybody techniques for real materials, quantum Monte Carlo, ab-initio molecular dynamics, electron-phonon coupling, large scale and multiscale simulations, activated processes, electronic transport, response to external fields, simulations in realistic environments.
- Applications: nanoscience, biochemistry and biomaterials, magnetism and spintronics, superconductivity, geophysics, functional materials, surfaces, spectroscopies, catalysis and electrochemistry, chemical reactions and kinetics, materials design.

Organizing committee

Ivo Souza (University of the Basque Country and Ikerbasque foundation)

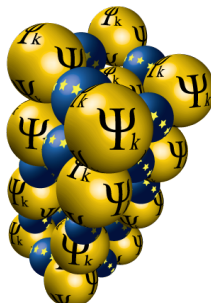
Ion Errea (University of the Basque Country)

Aran Garcia-Lekue (Donostia International Physics Center and Ikerbasque foundation)

Objectives

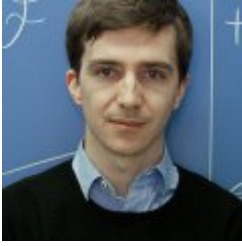
The main objective of this event is to identify new developments and topics in the field of electronic-structure methods from the first-principles perspective, their diverse applications, and its mathematical foundations. As such, it provides a great opportunity to assemble a wide range of leading scientists working on different aspects of computational material science.

Course specific contributors



HEZKUNTZA SAILA
DEPARTAMENTO DE EDUCACIÓN

Directed by



Ion Errea

UPV/EHU

After Ion Errea graduated, he started a PhD project supervised by Aitor Bergara and Vyacheslav Silkin at the University of the Basque Country (UPV/EHU) and the Donostia International Physics Center (DIPC). After defending his thesis he moved to the group of Francesco Mauri in the Institut de Minéralogie et de Physique des Milieux Condensés (IMPMC) at the Université Pierre et Marie Curie (UPMC) in Paris. His main task was to develop the Stochastic Self-Consistent Harmonic Approximation (SSCHA). In January 2014, he moved to the DIPC as a postdoctoral researcher to continue developing the SSCHA and applying it to systems of interests. Since April 2015 he is an Assistant Professor at the Department of Applied Physics 1 in the University of the Basque Country (UPV/EHU) and continues as an associate researcher of the DIPC.



Aran Garcia-Lekue

DIPC

Registration fees

REGISTRATION	UNTIL 08-01-2020
Regular attendant	100,00 EUR
Invited speaker / organizers	0 EUR

Place

Gipuzkoa