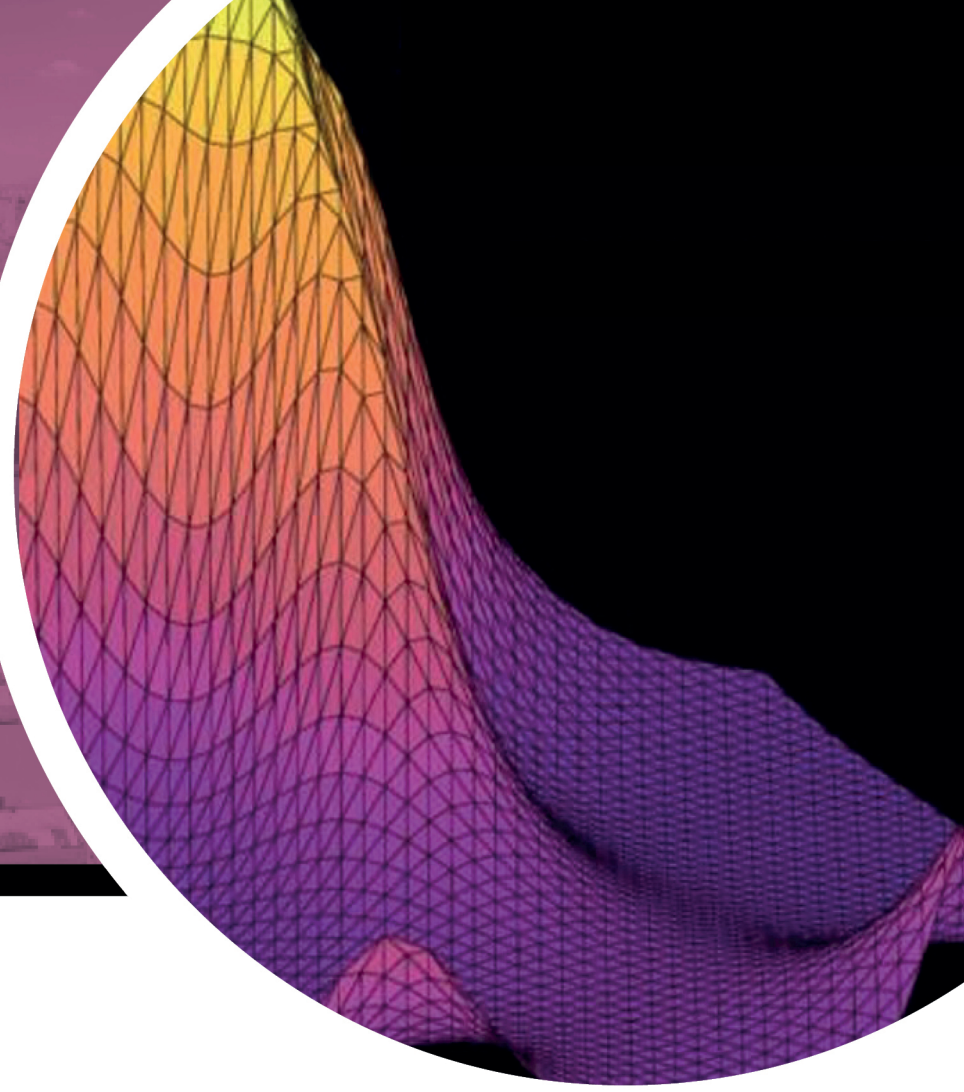
ICTP SAIFR | International Centre for Theoretical Physics | South American Institute for Fundamental Research

ICTP-SAIFR SCHOOL ON DFT AND BEYOND: ELECTRONIC STRUCTURE THEORY IN THE ERA OF DATA-DRIVEN SCIENCE



July 27 – August 7, 2020

IFT-UNESP Auditorium - São Paulo, Brazil

LECTURERS

Silvana Botti (Friedrich Schiller U. Jena, Germany)
Volker Blum (Duke U., USA)
Klaus Capelle (UFABC, Brazil)
Christian Carbogno (FHI, Germany)
Michele Ceriotti (EPFL, Switzerland)
Gustavo Dalpian (UFABC, Brazil)
Maurice de Koning (UNICAMP, Brazil)
Luca Ghiringhelli (FHI, Germany)
Dorothea Golze (Aalto U., Finland)
Oliver Hofmann (Technical U. Graz, Austria)
Angela Klautau (UFPA, Brazil)
Miguel Marques (U. of Halle, Germany)
Luana Pedroza (UFABC, Brazil)
Patrick Rinke (Aalto U., Finland)
Alexandre Rocha (IFT-UNESP, Brazil)
Mariana Rossi (FHI/MPSD, Germany)
Matthias Scheffler (FHI, Germany)
Alex Tkatchenko (U. of Luxembourg)
Weitao Yang (Duke U., USA)

Computational studies of molecules and condensed matter with ab initio electronic structure theory, i.e. computational materials science, aims to explore the huge uncharted territory of the chemical and structural space of materials. By doing so, it addresses current global challenges like the quest for efficient and sustainable use of energy resources. Besides its traditional role in interpreting experimental results, the accuracy of these methods also allows for predicting and designing new materials. As such, understanding and being able to run reliable first-principles simulations has become indispensable for condensed-matter physicists, chemists, and materials scientists of the present generation.

In this Hands-On school, senior experts and young specialists will give a comprehensive and pedagogical introduction on the fundamental principles and the cutting-edge theories in the areas of electronic structure theory, ab initio molecular dynamics, and machine learning applied to chemical physics and material science. Practical hands-on tutorials and Q&A sessions will ensure that different topics of interest can be discussed. The main computational workhorse for the afternoon sessions will be the FHI-aims all-electron code and codes connected to it. The overall school, however, is not designed to teach a single code, but rather to introduce scientific concepts.

There is no registration fee and limited funds are available for travel and local expenses.

Application deadline

May 2, 2020

Online registration form and information:

http://www.ictp-saifr.org/dft2020

FAPESP | ICTP | unesp | IFT - UNESP | FRITZ-HABER-INSTITUT MAX-PLANCK-GESELLSCHAFT | MS1P Molecular Simulations from First Principles

ORGANIZERS
Carsten Baldauf (FHI/U. Leipzig, Germany)
Adalberto Fazzio (LNNANO/CNPEM, Brazil)
Luana Pedroza (UFABC, Brazil)
Alexandre Rocha (IFT-UNESP, Brazil)
Mariana Rossi (FHI/MPSD, Germany)
Matthias Scheffler (FHI, Germany)