

# MaX School on Advanced Materials and Molecular Modelling with Quantum ESPRESSO



**17 - 28 May 2021**  
**An ICTP Virtual Meeting**  
**Trieste, Italy**

Further information:  
<http://indico.ictp.it/event/9616/>  
[smr3622@ictp.it](mailto:smr3622@ictp.it)

The school will introduce students and young researchers to materials and molecular modelling with Quantum ESPRESSO (QE), covering basic concepts, recent advances and developments, with emphasis on density-functional-theory (DFT) based methods and High-Performance Computing (HPC).

## Description:

Computational methods in electronic structure theory are a powerful tool for the understanding and the prediction of materials properties at the atomistic level. The combination of the progresses made by condensed matter theory with the increasing computing capabilities provided in HPC centers foster a great interest in computational materials science. Ab-initio electronic structure software like QE makes easily available such potentialities to a wide audience of scientists and students.

The school aims to train beginners in computational materials sciences to the efficient use of QE on modern massively parallel architectures, with special emphasis on the emerging architectures based on GPGPUs and on the use of advanced tools for generating, managing, storing, and sharing results.

## Directors:

S. BARONI, SISSA, Italy  
R. GEBAUER, ICTP, Italy  
A. KOKALJ, Jožef Stefan Institute, Slovenia  
W. REN, Shanghai University, China  
A. STROPPIA, CNR-SPIN, Italy

## Local Organiser:

I. GIOTTO, ICTP, Italy  
I. CARNIMEO, SISSA, Italy

## Keynote Speakers:

S. BLÜGEL, Peter Grünberg Institut and Institute for Advanced Simulation, Germany  
R. CAR, Princeton University, USA  
F. MAURI, Sapienza University of Rome, Italy  
N. SPALDIN, ETH Zurich, Switzerland  
X. GONG, Fudan University, China

## Lecturers:

M. BERCX, EPFL, Switzerland  
P. BONFA', University of Parma, Italy  
S. DE GIRONCOLI, SISSA, Italy  
P. DELUGAS, SISSA, Italy  
P. GIANNOZZI, University of Udine, Italy  
S. SCANDOLO, ICTP, Italy  
I. TIMROV, EPFL, Switzerland

## Hands-on Lecturers:

A. P. SEITSONEN, École Normale Supérieure Paris, France  
O. BASEGGIO, SISSA, Italy  
R. BERTOSSA, SISSA, Italy  
A. URRU, ETH, Switzerland

## Tutors:

F. CONTE, University of Naples, Italy  
P. CHANDRAMATHY SURENDRAN, Cochin University of Science and Technology, India  
Y. CUI, SHU EDU, China  
F. DOS SANTOS, EPFL, Switzerland  
M. HUŠ, National Institute of Chemistry, Ljubljana, Slovenia  
T. JIANG, SHU EDU, China  
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D. TISI, SISSA, Italy  
N. VELANKANNI, ICTP, Italy

## How to apply:

Online application:  
<http://indico.ictp.it/event/9616/>

Female scientists are encouraged to apply.

## Registration:

There is no registration fee.

## Deadline:

**30 April 2021**



The Abdus Salam  
**International Centre  
for Theoretical Physics**  
[www.ictp.it](http://www.ictp.it)  
Trieste, Italy

