



The Abdus Salam  
**International Centre  
for Theoretical Physics**



# Joint ICTP MARVEL College: Materials Simulation in the Age of AI

## DESCRIPTION:

This is a two-week intensive college on electronic-structure and atomistic simulations to understand, predict, and design the properties of materials. Foundational topics cover first-principles methods, molecular dynamics and machine-learning approaches, with lectures and hands-on sessions.

## TOPICS:

- Density-functional theory (DFT) and beyond
- Linear response and lattice dynamics (DFPT, phonons)
- Electronic, vibrational and core-level spectroscopies
- Many-body perturbation theory (GW, BSE)
- Topology and polarization (Berry phases, Wannier functions)
- Advanced functionals (Hubbard, Koopmans)
- Introduction to statistical sampling by molecular dynamics
- Sampling of different ensembles (thermostats, barostats, replica exchange)
- Rare events and enhanced sampling (metadynamics, accelerated MD)
- Machine learning for materials (descriptors, potentials, training and validation)
- Advanced ML for sampling (fine tuning, direct force prediction, force-free integration)

## MORE INFORMATION:

The Joint ICTP–MARVEL college brings together graduate students and early-career researchers to learn the state-of-the-art for computational materials science in the age of AI.

Week 1 focuses on electronic-structure theory and spectroscopies (density-functional theory and density-functional perturbation theory, many-body perturbation theory, topology and Wannier functions, advanced functionals).

Week 2 covers statistical mechanics and atomistic simulation, including enhanced sampling and machine-learning interatomic potentials. Hands-on labs deploy open source community codes, with poster sessions and open-mic discussions.

## SPEAKERS:

C. Clementi, Free University of Berlin, Germany  
C. Dellago, University of Vienna, Austria  
G. Galli, University of Chicago, USA

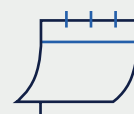
G. Kresse, University of Vienna, Austria  
M. Rossi, University of Cambridge, UK

## LECTURERS:

S. Baroni, SISSA, Italy  
G. Bussi, SISSA, Italy  
M. Calandra, University of Trento, Italy  
M. Cococcioni, University of Pavia, Italy  
N. Colonna, Paul Scherrer Institute, Switzerland  
S. De Gironcoli, SISSA, Italy  
P. Delugas, SISSA, Italy  
A. Ferretti, CNR, Italy  
R. Gebauer, ICTP, Italy  
P. Giannozzi, University of Udine, Italy  
A. Hassanali, ICTP, Italy

A. Laio, SISSA, Italy  
E. Linscott, Paul Scherrer Institute, Switzerland  
A. Marrazzo, SISSA, Italy  
L. Monacelli, Sapienza University of Rome, Italy  
S. Narasimhan, JNCASR, India  
M. Palummo, Tor Vergata University of Rome, Italy  
R. Resta, University of Trieste, Italy  
I. Souza, University of the Basque Country, Spain  
I. Timrov, Paul Scherrer Institute, Switzerland  
D. Varsano, CNR, Italy

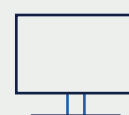
Poster sessions will take place in both week 1 and week 2.  
Applicants are welcome to submit an abstract.



**1-12 June 2026**



**Trieste, Italy**



## Applications and Deadlines:

**22 February 2026**  
for applicants needing visa support

**27 March 2026**  
for all other applicants

## DIRECTORS:

S. Bonella, CECAM, EPFL-Lausanne, Switzerland  
M. Ceriotti, EPFL-Lausanne, Switzerland  
N. Marzari, EPFL-Lausanne, Switzerland  
S. Scandolo, ICTP, Italy

## LOCAL ORGANIZER:

S. Scandolo, ICTP, Italy

## FURTHER INFORMATION:

E-mail: [smr4220@ictp.it](mailto:smr4220@ictp.it)

Web: <https://indico.ictp.it/event/11146/>

Female scientists are encouraged to apply.



## GRANTS:

A significant number of grants (travel and lodging, or only lodging) are available to support participants. There is no registration fee.

