

# ICTP-SISSA-CECAM Workshop on Molecular Dynamics and its Applications to Biological Systems



**21 - 25 September 2020**  
**An ICTP Virtual Meeting**  
**Trieste, Italy**

Further information:  
<http://indico.ictp.it/event/9128/>  
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There continues to be a growing community of scientists in both the developed and developing world, interested in and working on applications of molecular dynamics techniques to understand biological systems. This is highly relevant for problems in health and medicine.

## Description:

The topics of this workshop are relevant in diverse contexts, from basic science, where molecular modelling and simulations have become indispensable tools even to interpret and design experiments, to applicative avenues such as health and medicine where advanced MD simulation techniques are used for insilico drug screening. This workshop is aimed at bringing together world experts working in a broad range of topics related to bio-molecular simulations which will expose both young and advanced researchers to the state-of-the-art in the field.

## Topics:

- Quantum Mechanics in Biology: Enzyme Catalysis
- Protein Dynamics/Protein Folding
- Drug Design
- Protein Structure Prediction
- DNA/RNA Dynamics/Folding
- Coarse-grain simulations of nucleic acids & chromatin
- Multi-scale computer simulations for polymer melts
- Spectroscopy: Excited State Dynamics in Biology
- Stochastic processes in biophysics

## Directors:

G. BUSSI, SISSA  
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C. MICHELETTI, SISSA  
A. RODRIGUEZ, ICTP  
E. ROLDAN, ICTP  
A. ROSA, SISSA

## Local Organizer:

A. HASSANALI, ICTP

## Speakers:

M. BONOMI, Institut Pasteur - CNRS, France  
M.E. CASIDA, University of Grenoble, France  
M. CERIOTTI, Swiss Federal Institutes of Technology Lausanne (EPFL), Switzerland  
B. CHENG, Trinity College Cambridge University, UK  
G. COLOMBIO, Università di Pavia, Italy  
M. DE VIVO, Istituto Italiano di Tecnologia, Italy  
R. EICHHORN, The Nordic Institute for Theoretical Physics, Sweden  
R. EVERAERS, École Normale Supérieure de Lyon, France  
G. HUMMER, Max Planck Institute of Biophysics, Germany  
V. KAILA, Stockholm University, Sweden  
L. KAMMERLIN, Uppsala Biomedical Center, Sweden  
S. KHALID, University of Southampton, UK  
E. ROSTA, King's College London, UK  
L. ROVIGATTI, Sapienza University of Rome, Italy  
K. SEKIMOTO, Université Paris Diderot, France  
S. WOLF, Albert Ludwigs University, Germany

## How to apply:

Online application:  
<http://indico.ictp.it/event/9128/>

Female scientists are encouraged to apply.

## Deadline:

**14 September 2020**



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