

# Conference on Frontiers in Atomistic Simulations: from Physics to Chemistry and Biology

## Description:

This workshop gathers global experts to advance atomistic simulation methods and explore frontier applications in physical and chemical sciences. It features an interdisciplinary mix of topics, including physics, chemistry, biology, and engineering, fostering collaboration and innovation.

## TOPICS:

- Classical and First Principles Molecular Dynamics to study complex chemical and biological problems ranging from chemistry at interfaces to enzyme catalysis in proteins and drug discovery
- Methods Development in Enhanced Sampling/Rare events
- Application of Enhanced Sampling Methods to tackle complex problems in physics, chemistry and biology
- Development and Application of Machine Learning Potentials
- Machine-Learning techniques for automatic/agnostic discovery of reaction coordinates/order parameters

## PRELIMINARY LIST OF SPEAKERS:

Narjes Ansari, Qubit Pharmaceutical  
Alessandro Barducci, CNRS  
Stefano Baroni, SISSA  
Joerg Behler, Bochum  
Marco Bernasconi, U Milano-Bicocca  
Mauro Boero, CNRS-Strasbourg  
Luigi Bonati, IIT  
Max Bonomi, CNRS  
Roberto Car, Princeton  
Andrea Cavalli, CECAM, EPFL  
Matteo Ceccarelli, U Cagliari  
Michele Ceriotti, EPFL  
Jayashrita Debnath, MPI  
Cristoph Dellago, U Vienna  
Davide Donadio, UC Davis  
Laura Gagliardi, Chicago  
Vanda Glezakou, Oak Ridge National Lab  
Francois Gygi, UC Davis  
Barak Hirshberg, Tel Aviv University  
Tarak Karmakar, IIT New Delhi  
Michael Klein, Temple  
Jorge Kohanoff, Universidad Politecnica de Madrid  
Zhipan Liu, Fudan  
Roman Martonak, Univerzita Komenského v Bratislave

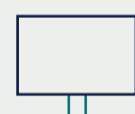
Carla Molteni, Kings College London  
Chris Mundy, PNNL  
Hayiang Niu, NPU  
Simona Parrinello, UCL  
Daniele Passerone, EMPA  
Pablo Piaggi, CIC nanoGUNE  
Giovanni Maria Piccini, U Modena  
Maria Ramos, U Porto  
Umberto Raucci, IIT  
Simone Raugei, PNNL  
Dhiman Ray, U Oregon  
Valerio Rizzi, U Geneva  
Ursula Roethlisberger, EPFL  
Roger Rousseau, Oak Ridge National Lab  
Angel Rubio, Flatiron Institute, Max-Planck Hamburg  
Matteo Salvalaglio, UCL  
Annabella Selloni, Princeton  
Michiel Sprik, Cambridge  
Pratyush Tiwary, U Maryland  
Gareth Tribello, Queens Belfast University  
Omar Valsson, U North Texas  
Greg Voth, U Chicago  
Wan-Jian Yin, Soochow University



**8 - 12 September 2025**



**Trieste, Italy**



**Deadline:  
30 June 2025**

## DIRECTORS:

Giovanni Bussi, SISSA  
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Alessandro Laio, SISSA  
Vittorio Limongelli, USI Lugano  
Carmen Rovira, University of Barcelona,  
Erio Tosatti, ICTP & SISSA

## LOCAL ORGANISER:

Ali Hassanali, ICTP

## FURTHER INFORMATION:

E-mail: [smr4098@ictp.it](mailto:smr4098@ictp.it)  
Web: <http://indico.ictp.it/event/10863/>  
Female scientists are encouraged to apply.



## GRANTS:

A limited number of grants are available to support the attendance of selected participants, with priority given to participants from developing countries. There is no registration fee.

