



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



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 or 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 Rousseu, 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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Marco De Vivo, Istituto Italiano di Tecnologia
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Xingao Gong, Fudan University
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

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.



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