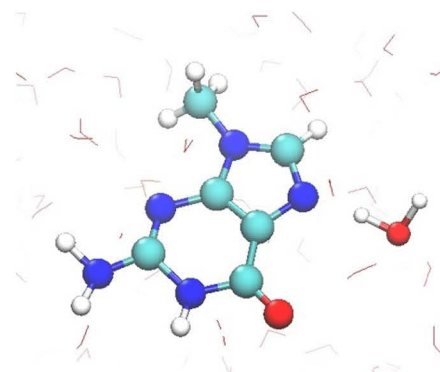




The Abdus Salam

**International Centre  
for Theoretical Physics**

[www.ictp.it](http://www.ictp.it)



*Conference on Atomistic Simulations of Biomolecules:  
towards a Quantitative Understanding of Life Machinery  
(6 - 10 March 2017)*

*Miramare - Trieste, Italy*

The Abdus Salam International Centre for Theoretical Physics (ICTP), Trieste, Italy is organizing a **Conference on Atomistic Simulations of Biomolecules: towards a Quantitative Understanding of Life Machinery** to be held in Trieste, Italy from **6 - 10 March 2017**.

In the last decades accurate atomistic simulations have become a key tool for studying biomolecules and is an essential part of quantitative life sciences. Thanks to specialized hardware, distributed computing and enhanced sampling techniques, the timescales that can be reached by simulations and the shortest timescales that can be probed experimentally are now overlapping. Besides providing more benchmarks with which theoretical models can be validated, atomistic simulations give valuable information on microscopic details that help in the interpretation of experiments. It can be foreseen that in the near future, the scientific community will start trusting simulations as a genuinely predictive tool, whose outcome is valid even without direct experimental support. In the next years, simulations are likely to play a crucial role in understanding how life machinery works.

The scope of this conference is bringing together experts working in the field of atomistic simulations of biomolecules, with particular attention to exposing scientists working in developing countries to the state of the art methods and applications possible in the field. It will also serve to link together both students and faculty, to encourage involvement for exchange and collaboration.

**Topics will include:**

- 1) **Simulation of nucleic acids;**
- 2) **Protein folding and aggregation;**
- 3) **Molecular recognition;**
- 4) **The role of water in bio-molecular processes;**
- 5) **Algorithm development for enhanced sampling and multiscale simulations;**
- 6) **Force-fields for bio-molecular simulations.**

**GRANTS**

A limited number of grants are available to support the travel and living expenses of selected participants, with priority given to participants working in a developing country and who are at the early stages of their career.

**HOW TO APPLY FOR PARTICIPATION:**

The **application form** can be accessed at the activity website:

<http://indico.ictp.it/event/7610/>

Once in the website, comprehensive instructions will guide you step-by-step, on how to fill out and submit the application forms.

**DEADLINE for requesting participation:  
15 NOVEMBER 2016**

ICTP Secretary: Ms. Doreen M. Sauleek (smr2828)

Tel.: +39-040-2240346  
Fax: +39-040-224163

Trieste, July 2016

Email: [smr2828@ictp.it](mailto:smr2828@ictp.it)  
ICTP Home page: <http://www.ictp.it>



IAEA  
International Atomic Energy Agency

**ORGANIZERS:**

**Ali HASSANALI**  
ICTP, Trieste, Italy

**Lucy KIRURI**  
Kenyatta University,  
Nairobi, Kenya

**Alessandro LAIO**  
SISSA, Trieste, Italy

**Nina PASTOR**  
UAEM, Mexico

**TENTATIVE  
LIST OF SPEAKERS:**

**Robert BEST**  
NIH, Washington, U.S.A.

**Julio CABALLERO**  
Universidad de Talca, Chile

**Pilar COSSIO**  
MPI, Frankfurt, Germany

**Laura DOMINGUEZ**  
UNAM, Mexico

**Vanessa LEONE**  
University of Chicago, U.S.A.

**Kersten LINDORFF-LARSEN**  
University of Copenhagen,  
Denmark

**Sergio PANTANO**  
Institut Pasteur,  
Montevideo, Uruguay

**Sergiy PEREPELYTSYA**  
BITP, Kiev, Ukraine

**Meher PRAKASH**  
JNCASR, Bangalore, India

**Fabio STERPONE**  
IBPC-LBT, Paris, France

