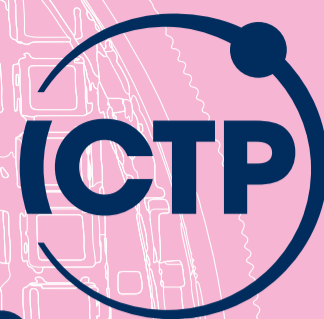


# Joint ICTP-IAEA School and Workshop on Fundamental Methods for Atomic, Molecular and Materials Properties in Plasma Environments



**16 - 20 April 2018**  
**Trieste, Italy**

Further information:

<http://indico.ictp.it/event/8305/>  
[smr3197@ictp.it](mailto:smr3197@ictp.it)

The Abdus Salam International Centre for Theoretical Physics (ICTP) and the International Atomic Energy Agency (IAEA) will jointly organize this School and Workshop on Fundamental Methods for Atomic, Molecular and Materials Properties in Plasma Environments.

## Directors:

B.J. BRAAMS, CWI, Amsterdam, Netherlands  
H.K. CHUNG, IAEA, Vienna, Austria  
G. CSÁNYI, University of Cambridge, U.K.  
A.G. CSÁSZÁR, MTA-ELTE Complex Chemical Systems Research Group,  
Budapest, Hungary  
A.I. KRYLOV, University of Southern California, Los Angeles, U.S.A.

## Local Organizer:

G. THOMPSON, ICTP, Trieste, Italy

## Description:

The one-week event at ICTP in Trieste will provide training and information exchange for computational scientists working on models and data for atomic, molecular and materials processes relevant to fusion energy research, industrial plasmas, laser-produced plasmas, astrophysical plasmas, and warm and hot dense matter. The training is aimed at advanced Ph.D. students, postdocs and other young researchers. The information exchange will span several disciplines: from molecules to materials and from method developments to data treatments. Topics related to energetic events and electronically excited states are emphasized throughout the programme. The schedule features lectures by international experts, invited and contributed research talks, posters and discussion sessions, with ample time available for interaction and discussions.

## Topics:

- Advanced electronic structure approaches. Equation-of-motion and other wavefunction-based methods for excited electronic states. Coupled cluster methods applied to solids. State-of-the-art methods for alloys and liquid metals. New developments based on reduced density matrices and the density matrix renormalization group.
- Nuclear quantum dynamics. Quantum treatments of scattering. Path integral molecular dynamics including treatment of multiple electronic surfaces. Determination of reaction rates beyond Arrhenius scaling.
- Potential energy and property surfaces. Machine-learning and kernel-based methods. Methods for multiple electronic states and their interactions.
- Uncertainty assessment and uncertainty propagation. Uncertainty correlations and other topics.
- Applications. Electronic and atomic collisions in plasmas. Plasma-material interaction and radiation damage of materials.

## Invited Speakers:

V. AVERBUCK, Imperial College London, U.K.  
A.D. BACZEWSKI, Sandia National Laboratory, Albuquerque, NM, U.S.A.  
K. BURKE, UC Irvine, CA, U.S.A.  
A. DE VITA, King's College London, U.K.  
W.M.C. FOULKES, Imperial College London, U.K.  
S. FRITZSCHE, GSI and Friedrich Schiller University, Jena, Germany  
C.H. GREENE, Purdue University, Lafayette, IN, U.S.A.  
M.P. HEAD-GORDON, UC Berkeley, CA, U.S.A.  
K. HEINOLA, University of Helsinki, Finland and CCFE/JET, U.K.  
T. HICKEL, MPIE, Düsseldorf, Germany  
T.-C. JAGAU, Ludwig-Maximilians-Universität, Munich, Germany  
J.R. KERMODE, Warwick University, U.K.  
J. KOHANOFF, Queen's University Belfast, U.K.  
N. MOISEYEV, Technion, Haifa, Israel  
T. ODA, Seoul National University, Seoul, Republic of Korea  
R. SANTRA, Center for Free-Electron Laser Science, Hamburg, Germany  
J.E. SUBOTNIK, University of Pennsylvania, Philadelphia, PA, U.S.A.  
J. TENNYSON, University College London, U.K.  
U. VON TOUSSAINT, IPP, Garching, Germany  
D.R. TRINKLE, University of Illinois, Urbana-Champaign, IL, U.S.A.  
G.A. WORTH, University College London, U.K.  
Z. ZENG, CAS Institute for Solid State Physics, Hefei, China  
P. ZHANG, Peking University and IAPCM, Beijing, China  
Z. ZHAO, National University of Defense Technology, Changsha, China  
B. ZIAJA-MOTYKA, DESY, Hamburg, Germany

## How to apply:

Online application:  
<http://indico.ictp.it/event/8305/>

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.

## Deadline:

**20 November 2017**



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

