The Abdus Salam
International Centre for Theoretical Physics

United Nations Educational, Scientific and Cultural Organization

IAEA International Atomic Energy Agency

ICTP-IAEA Workshop
Non-adiabatic dynamics and radiation damage in nuclear materials

14 – 18 November 2011

(Miramare - Trieste, Italy)

The Abdus Salam International Centre for Theoretical Physics is organizing an *ICTP-IAEA Workshop on Non-adiabatic dynamics and radiation damage in nuclear materials* to be held at ICTP, Trieste, Italy from 14 to 18 November 2011.

Understanding radiation damage is central to assess the durability of materials hosting nuclear waste and engineering materials for nuclear fusion/fission reactors. It is also crucial in other fields such as space electronics under cosmic radiation, novel processing techniques using lasers and ions, and irradiation on biological matter.

In the two extreme limits, the projectiles deposit their energy either into the electronic system, or into the nuclear degrees of freedom. However, in the general case, one has to consider the non-equilibrium coupled dynamics of nuclei (ions) and excited electrons. The past decades have seen a continuous attempt at understanding materials under irradiation via molecular dynamics (MD) simulations with empirical or semi-empirical potentials. More recently, ab initio calculations were used to compute properties like defect energies, and also to derive accurate force fields. However, except for a few notable exceptions, electronic excitations and the energy transfer between electrons and nuclei remained largely outside the framework.

The main aim of this Workshop is to put together experts in methods for coupled electron-ion dynamics, and experts in radiation effects to explore the potential of electronic structure based theoretical/computational approaches to understand irradiation of materials under extreme conditions. A further objective is to help bridge the gap between the highly efficient, large scale MD simulations and the more accurate but more expensive non-adiabatic MD, through exchange of ideas that could help in the development of new methods and algorithms.

The focus of the Workshop will be on theoretical approaches and computational methods. This will be complemented with talks describing the materials of interest and also talks on experiments and their connection with models. The scientific program will encompass the following topics:

- **Materials challenges in the nuclear industry. Fuels, waste, fission and fusion.**
- **Experimental techniques and connection with models and theory.**
- **Classical simulations of radiation cascades. Empirical potentials.**
- **Electronic structure: approximations, methods and codes.**
- **Dynamics of electrons and nuclei: TD-DFT, stopping, Ehrenfest dynamics.**
- **Linking electronic structure and force fields. Fitting potentials. Tight-binding.**
- **Two-temperature models. Thermal spike vs. Coulomb explosion.**
- **Beyond Ehrenfest. Electron-phonon interactions.**
- **Larger systems and longer time scales. Kinetic MC. Multiscale modeling.**

Participants are encouraged to present their work in a poster session. A limited number of these will be selected for a brief oral presentation

Participation

Applicants from all countries that are members of the United Nations, UNESCO or IAEA may attend. As the Workshop will be conducted in English, participants should have an adequate working knowledge of this language. Although the main purpose of the Centre is to help research workers from developing countries through a programme of training activities within a framework of international cooperation, a limited number of students and post-doctoral scientists from developed countries are also welcome to attend.

As a rule, travel and subsistence expenses of the participants should be borne by their home institutions. Every effort should be made by candidates to secure support for their fare (or at least half-fare). However, limited funds are available for some participants, who are nationals of, and working in, a developing country, and who are not more than 45 years old. Such support is available only to those attending the entire activity. *There is no registration fee*.

HOW TO APPLY FOR PARTICIPATION

The Online Application can be accessed at the activity website: *http://agenda.ictp.it/smr.php?2260*. Comprehensive instructions will guide you step-by-step on how to fill out and submit the application form. Kindly send all file attachments in Word or Acrobat format.

***Secretariat:* Ms. Rosa del Rio (smr 2260)**
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Organizers

Victor Inozemtsev
(IAEA, Vienna, Austria)

Jorge Kohanoff
(Queen's University Belfast, UK)

Local organizer

Sandro Scandolo
(ICTP, Trieste, Italy)

Speakers include

Emilio Artacho (Univ. of Cambridge, UK)
Mads Brandbyge (Technical Univ. Denmark)
Alfredo Caro (Los Alamos National Lab. USA)
Roberto Coppola (ENEA, Italy)
Ian Farnan (Univ. of Cambridge, UK)*
Andrew Fisher (Univ. College London, UK)*
Matthew Foulkes (Imperial College London,UK)
Lorenzo Malerba (SKC.CEN, Belgium)*
Alexander Ryazanov (Kurchatov Inst. Russia)
Alexander Solontsov (Bochvar Inst. Russia)
Maximo Victoria (LLNL, USA&CIEMAT, Spain)
François Willaime (CEA Saclay, France)

****to be confirmed***

DEADLINE

for requesting participation

3 July 2011

(if financial support and/or visa are needed)

18 September 2011

(if neither financial support nor visa are needed)