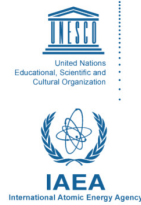




The Abdus Salam  
International Centre for Theoretical Physics



## Joint ICTP-IAEA Workshop on Non-adiabatic Dynamics and Radiation Damage in Nuclear Materials

Organizer(s): IAEA: V. Inozemtsev. Queen's University, Belfast: J. Kohanoff. ICTP: S. Scandolo  
Trieste - Italy, 14 - 18 November 2011

Venue: Leonardo da Vinci Building Euler Lecture Hall

### Final programme

Monday, 14 November 2011 (Room:Leonardo da Vinci Building Euler Lecture Hall)

- 09:00 - 10:00** (Room: Leonardo da Vinci Building, Lobby)  
--- Registration and administrative formalities ---
- 10:00 - 11:00** **V. Inozemtsev (IAEA), S. Scandolo (ICTP)**  
**Introduction and opening**
- 11:00 - 11:30** --- Coffee break ---
- 11:30 - 12:30** **I. Farnan / Univ. Cambridge, UK**  
**Experimental quantification of radiation damage in ceramics**
- 12:30 - 14:00** --- Lunch break ---
- 14:00 - 15:00** **J. Kohanoff / Queen's Univ. Belfast, UK**  
**Electronic structure: basics and DFT**
- 15:00 - 15:30** **E. Artacho / Univ. Cambridge, UK**  
**Time-evolving TD-DFT for time-dependent electronic problems**
- 15:30 - 16:00** **A. Caro / Los Alamos National Lab., USA**  
**Materials challenges in the nuclear industry: steels**
- 16:00 - 16:30** --- Coffee break ---

16:30 - 17:30 **A. Caro / Los Alamos National Lab., USA**  
**Empirical force fields for nuclear materials**

**Tuesday, 15 November 2011 (Room:Leonardo da Vinci Building Euler Lecture Hall)**

09:00 - 10:00 **F. Willaime / CEA Saclay, France**  
**Introduction to Molecular Dynamics simulations**

10:00 - 11:00 **M. Victoria / Univ. Politecnica Madrid, Spain**  
**An introduction to radiation damage physics**

11:00 - 11:30 --- Coffee break ---

11:30 - 12:30 **A. Caro / Los Alamos National Lab., USA**  
**The electron-phonon problem in metals**

12:30 - 14:00 --- Lunch break ---

14:00 - 15:00 **M. Foulkes / Imperial College London, UK**  
**Electronic stopping: background and simulation methods**

15:00 - 16:00 **E. Artacho / Univ. Cambridge, UK**  
**Stopping power of projectiles shooting through materials: Predicting the rate of electron heating in radiation damage events**

16:00 - 16:30 --- Coffee break ---

16:30 - 17:30 **F. Willaime / CEA Saclay, France**  
**Electronic structure calculations in materials for nuclear energy**

19:30 - 21:30 --- Welcome Reception ---

**Wednesday, 16 November 2011 (Room:Leonardo da Vinci Building Euler Lecture Hall)**

09:00 - 10:00 **M. Victoria / Univ. Politecnica Madrid, Spain**  
**Experimental validation of radiation damage models**

10:00 - 11:00 **M. Foulkes / Imperial College London, UK**  
**Tight-binding Ehrenfest molecular dynamics studies of electronic stopping in metals**

11:00 - 11:30 --- Coffee break ---

11:30 - 12:30 **R. Coppola / ENEA-Casaccia, Rome, Italy**  
**Applications of small-angle neutron scattering (SANS) in the microstructural investigation of irradiated nuclear steels**

12:30 - 14:00 --- Lunch break ---

14:00 - 15:00 **A. Ryazanov / Kurchatov Institute, Moscow, Russia**  
**Theoretical modeling of the influence of swift heavy ion irradiation on materials: thermal spike vs. Coulomb explosion**

- 15:00 - 16:00**     **E. Bringa** / *Univ. Nacional de Cuyo Mendoza, Argentina*  
**Atomistic simulations of radiation effects in the electronic regime**
- 16:00 - 16:30**     --- Coffee break ---
- 16:30 - 17:00**     **J. Kohanoff** / *Queen's Univ. Belfast, UK*  
**Electronic structure: computational methods**
- 17:00 - 17:30**     **A. Correa** / *Lawrence Livermore National Laboratory, USA*  
**Electronic stopping power with TDDFT: From dielectric models to real time propagators**
- 17:30 - 19:00**     (Room: Leonardo da Vinci Building, Lobby)  
**Poster session**

**Thursday, 17 November 2011** (Room:Leonardo da Vinci Building Euler Lecture Hall)

- 09:00 - 10:00**     **A. Solontsov** / *State Center for Condensed Matter Physics, Moscow, Russia*  
**Nonlinear magnetic dynamics and fluctuations**
- 10:00 - 11:00**     **A. Ryazanov** / *Kurchatov Institute, Moscow, Russia*  
**Charge state effects of radiation damage on microstructure evolution in dielectric materials under neutron and charged particle irradiation**
- 10:30 - 11:00**     --- Coffee break ---
- 11:30 - 12:00**     **T. Apostolova** / *Institute for Nuclear Research and Nuclear Energy, Sofia, Bulgaria*  
**Modeling of the electronic dynamics in swift heavy ion irradiated semiconductor materials**
- 12:00 - 12:30**     **D. Nicholson** / *Oak Ridge National Laboratory, USA*  
**Calculated Magnetic Structure in Irradiated Fe**
- 12:30 - 14:00**     --- Lunch break ---
- 14:00 - 15:00**     **A. Fisher** / *University College London, UK*  
**Why go beyond Ehrenfest? Two-way energy transfer between electrons and ions**
- 15:00 - 16:00**     **J. Lu** / *Technical University of Denmark*  
**A Langevin approach to nonadiabatic molecular dynamics**
- 16:00 - 16:30**     --- Coffee break ---
- 16:30 - 17:30**     **A. Solontsov** / *State Center for Condensed Matter Physics, Moscow, Russia*  
**Excitations of the electron Fermi liquid**

**Friday, 18 November 2011** (Room:Leonardo da Vinci Building Euler Lecture Hall)

- 09:00 - 10:00**     **A. Fisher** / *University College London, UK*  
**A route beyond Ehrenfest: Correlated electron-ion dynamics**
- 10:00 - 11:00**     **L. Stella** / *Univ. del Pais Vasco San Sebastian, Spain*  
**Correlated Electron-Ion Dynamics for resonant systems: High order expansion and applications to simple models**

- 11:00 - 11:30**     **P. W. Ma (Culham Science Centre, , UK) & E. Semenov (Kurchatov Institute, Russia)**  
**Presentations by participants**
- 11:30 - 12:00**     --- Coffee break ---
- 12:00 - 12:30**     **L. Malerba / *SKC.CEN, Belgium***  
**Radiation damage in structural materials for GenIV and fusion reactors**
- 12:30 - 13:00**     **L. Malerba / *SKC.CEN, Belgium***  
**Beyond the displacement cascade: Nanostructural evolution in metals under irradiation and correlation with mechanical properties**
- 13:00 - 13:30**     **Closing, Round table discussion. Challenges ahead.**