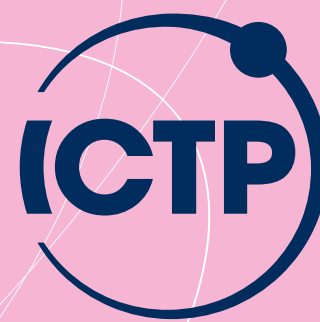


# Joint ICTP-IAEA Virtual Workshop on Atomistic Modelling of Radiation Damage in Nuclear Systems

**4 - 8 October 2021**  
**An ICTP Virtual Meeting**  
**Trieste, Italy**



Further information:  
<http://indico.ictp.it/event/9547/>  
[smr3573@ictp.it](mailto:smr3573@ictp.it)

This virtual workshop will assist Ph.D. students and early-career researchers in developing a qualitative and quantitative understanding of the atomistic modelling of radiation damage on materials, both for existing fission and proposed fusion reactors.

## Description:

Atomistic modelling is the simulation of the behaviour of complex systems by explicitly taking its smallest constituent parts into account. In the context of radiation damage in nuclear materials, these simulations involve the bulk and surface atoms of reactor components and their interactions with energetic neutrons and plasma in the form of free atoms, molecules and ions. The computational techniques employed include molecular dynamics, rate theory equations, density functional theory, and a variety of Monte Carlo methods; this Workshop provides an introduction to some popular software used to implement these techniques, with practical sessions on the free packages LAMMPS and SRIM.

## Topics:

- Irradiated material: defect and cascade production
- Damage dose-rate, energies, and atomic displacement
- Neutron-induced material defect simulation
- Theoretical modelling of radiation effects
- Plasma-surface interaction: erosion and surface-evolution studies
- Hydrogen isotope deposition, trapping and permeation in fusion-relevant materials

## Directors:

K. HEINOLA, IAEA, Austria  
C. HILL, IAEA, Austria  
J. C. SUBLET, IAEA, Austria

## Local Organiser:

N. SERIANI, ICTP, Italy

## Speakers:

T. AHLGREN, University of Helsinki, Finland  
M. J. CATURLA, University of Alicante, Spain  
P. DERLET, Paul Scherrer Institute, Switzerland  
F. GRANBERG, University of Helsinki, Finland  
D. MASON, UKAEA, UK  
A. SAND, Aalto University, Finland  
K. SCHMID, Max Planck Institute for Plasma Physics, Germany  
U.V. TOUSSAINT, Max Planck Institute for Plasma Physics, Germany

## How to apply:

Online application:  
<http://indico.ictp.it/event/9547/>

Female scientists are encouraged to apply.

## Registration:

There is no registration fee.

## Deadline:

**19 September 2021**

