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

4 – 8 October 2021

Virtual Meeting

AGENDA

Monday, 4 October 2021

14:00 – 14:30 Opening, welcome and introductions; administrative details

14:30 – 15:30 **Andrea SAND**, *Aalto University, Finland*
Molecular Dynamics simulations of Collisional Cascades

15:30 – 16:30 **María J. CATURLA**, *Department of Applied Physics, University of Alicante, Spain*
Molecular Dynamics simulations of Collisional Cascades

16:30 – 17:00 Computing practicals: technical briefing

Tuesday, 5 October 2021

14:00 – 15:00 **Fredric GRANBERG**, *Department of Physics, University of Helsinki, Finland*
High-dose simulations of radiation damage in nuclear materials

15:00 – 17:00 LAMMPS Molecular Dynamics practical: cascade formation in bulk tungsten at moderate PKA energies

Wednesday, 6 October 2021

14:00 – 16:00 Poster Session and contributed talks

16:00 – 17:00 **Daniel MASON**, *Culham Centre for Fusion Energy, United Kingdom*
Now plot the graph: finding quantitative data from atomic configurations

The Abdus Salam International Centre for Theoretical Physics

IAEA International Atomic Energy Agency
Atoms for Peace and Development

Thursday, 7 October 2021

14:00 – 15:00 **Klaus SCHMID**, *Max Planck Institute for Plasma Physics, Garching, Germany*
Modeling the transport of fast ions in matter

15:00 – 17:00 SDTRIM 6.0 practical: self-ion implantation and sputtering for tungsten

Friday, 8 October 2021

14:00 – 15:00 **Peter DERLET**, *Paul Scherrer Institute, Switzerland*
The Creation Relaxation Algorithm (CRA): emergent microstructure in the high-dose irradiation regime

15:00 – 16:00 **Tommy AHLGREN**, *Department of Physics, University of Helsinki, Finland*
Rate equation simulations of defects in solids

16:00 – 17:00 Question and Answer session