

The IAEA

- Founded in 1957 to pursue the “safe, secure and peaceful uses of nuclear sciences and technology”.
- Autonomous, but reports to the UN General Assembly and Security Council. 173 Member States.
- Missions:
 - Safeguards
 - Nuclear safety
 - Peaceful uses of nuclear technology



The Atomic and Molecular Data Unit

- Founded in 1977 to “Stimulate international cooperation in measurement, compilation and evaluation of A+M / PSI data for fusion”.
- Atomic, Molecular and Plasma-Surface Interaction data.
- Five staff members:
 - Christian Hill (Unit Head)
 - Kalle Heinola (Atomic Physicist)
 - Ludmila Maria (Scientific Data Manager)
 - Marco Verpelli (Nuclear Data Analyst / Programmer)
 - Dipti (SSA Consultant: Atomic Collisional Data)

<https://amdis.iaea.org>

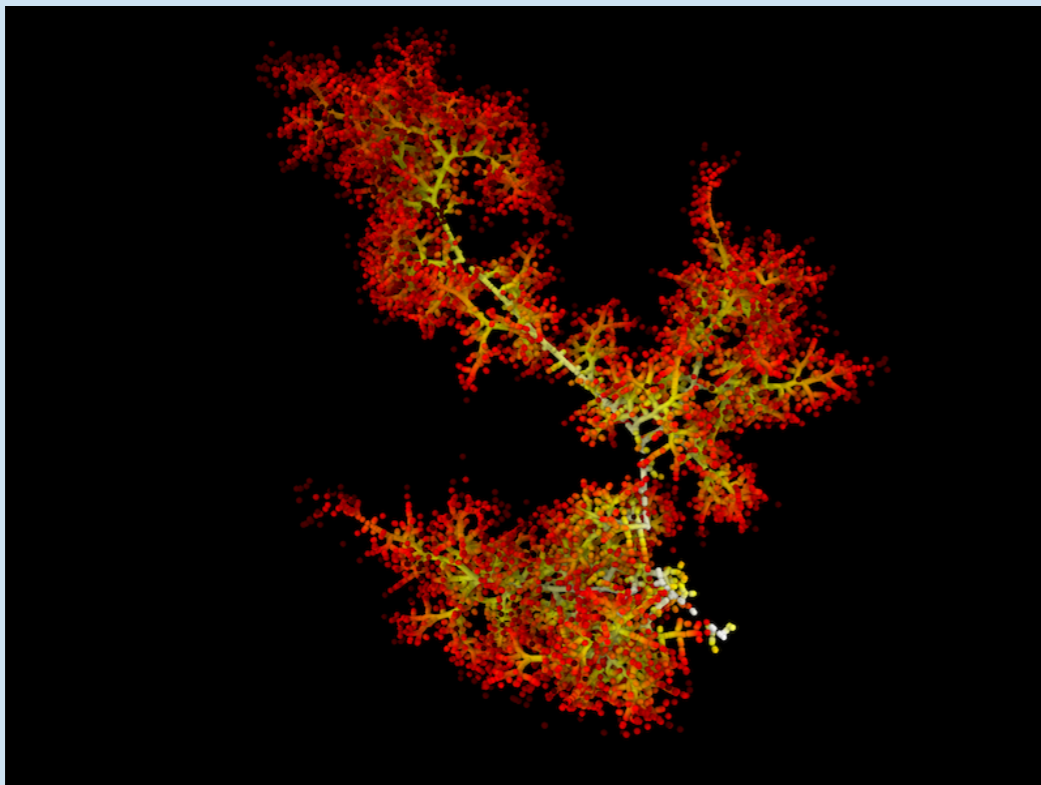
Activities: Coordinated Research Projects

- 3 – 5 Years
 - 8 – 15 Laboratories
 - 3 Research Coordination Meetings (RCMs)
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- Data for Erosion and Tritium Retention in Beryllium Plasma-Facing Materials
 - Plasma-wall Interaction with Irradiated Tungsten and Tungsten Alloys in Fusion Devices
 - Plasma-wall Interaction with Reduced-Activation Steel Surfaces in Fusion Devices
 - **Hydrogen Permeation in Nuclear Materials**

Databases

- CascadesDB
 - Molecular dynamics simulations of collision cascades for modelling radiation damage ...
 - This afternoon's lectures...
 - 814 GB of data in 14382 simulations across 293 archives
 - <https://cascadesdb.iaea.org/>

Cascade in tungsten from 200 keV PKA (A. Sand)



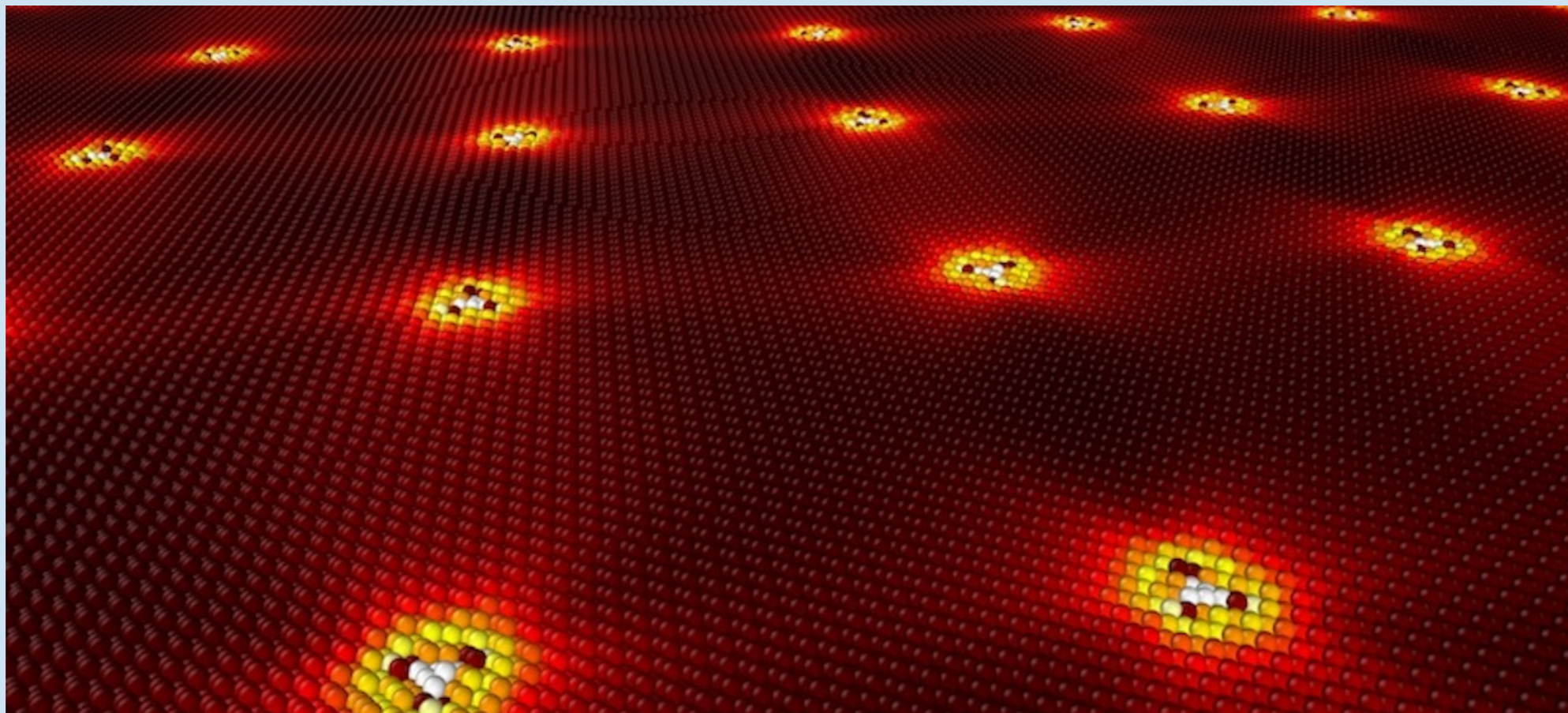
Analysis of defect structures with CSaransh (U. Bhardwaj)



Databases

- DefectDB
 - DFT calculations of radiation-induced defect structures in nuclear materials
 - Under development
 - <https://db-amdis.org/defectdb/>

A periodic network of screw dislocations in bcc Fe (A. Goryaeva and M.-C. Mărinică)



This Workshop

- <https://amdis.iaea.org/workshops/ictp-2021>
- <https://indico.ictp.it/event/9547/>
- Lectures and Computing Practicals:
 - Molecular Dynamics (MD) simulations
 - Connecting MD simulations to experiment through Kinetic Monte Carlo techniques
 - Contributed talks (10') and Posters (flash presentations: 2–3')
 - Characterising thermomechanical properties from MD simulations
 - Modelling fast ion transport in nuclear materials (SDTRIM)
 - Studies of microstructure evolution under high-dose irradiation
 - Rate equation simulations of defects
 - Q & A Session (Friday)

Contact email address: smr3573@ictp.it