

# **MoD-PMI 2025**

**Monday 26 May 2025 - Wednesday 28 May 2025**

**IAEA  
Programme**

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# Monday 26 May 2025

## Welcome - Press Room (09:15 - 09:35)

## invited - Press Room (09:35 - 10:35)

time	title	presenter
09:35	Alternative plasma facing material for nuclear fusion reactors	GONZALEZ-ARRABAL, Raquel (Universidad Politécnica de Madrid)
10:05	Experiments and modeling of hydrogen isotope inventory in damaged tungsten	KOBAYASHI, Makoto (National Institute for Fusion Science)

## contributed - Press Room (10:35 - 10:55)

## invited - Press Room (11:25 - 12:55)

time	title	presenter
11:25	A foundation model for atomistic materials chemistry	CSANYI, Gabor (University of Cambridge)
11:55	From Grains to Gigabytes: Generating Massive Virtual Specimens for Irradiation Damage Study	SHIN, Younggak (Yonsei University)
12:25	Point-Defect-Induced Metastable Phase Diagrams	NASTAR, Maylise (CEA)

## contributed - Press Room (12:55 - 13:15)

time	title	presenter
12:55	Microstructure impact on tritium retention and permeation in tungsten/oxide interface from first-principles based phase field modelling	NGUYEN-MANH, Duc (United Kingdom Atomic Energy Authority)

## lunch (13:15 - 14:30)

## invited - Press Room (14:30 - 15:30)

time	title	presenter
14:30	Detection of defects in displacement-damaged tungsten and iron	MARKELJ, Sabina (Jozef Stefan Institute)
15:00	Positron Annihilation Spectroscopy for vacancy defects studies in irradiated tungsten: Combination of modelling and experiments for vacancy size distribution and impurities interaction determination	BARTHE, Marie-France (CNRS)

## contributed - Press Room (15:30 - 15:50)

## invited - Press Room (15:50 - 16:15)

time	title	presenter
15:50	Positron Annihilation Spectroscopy for vacancy defects studies in irradiated tungsten: Combination of modelling and experiments for vacancy size distribution and impurities interaction determination	BARTHE, Marie-France (CNRS)

15:30	Impact of the trapping model on Tritium retention and permeation in DEMO Tungsten/Eurofer First Wall	HODILLE, Etienne (CEA-IRFM, F-13108 Saint Paul Lez Durance, France)
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**break - Press Room (15:50 - 16:20)****invited - Press Room (16:20 - 17:20)**

time	title	presenter
16:20	Adsorption and in-diffusion of Hydrogen at metal and metal oxide surfaces	FUKUTANI, Katsuyuki (University of Tokyo)
16:50	Interface-induced enhanced deuterium plasma-driven permeation in chemical vapor deposition tungsten-copper composite	CHENG, Long (Beihang University)

# Tuesday 27 May 2025

## invited - Press Room (09:00 - 10:00)

time	title	presenter
09:00	Quantum-accurate large-scale atomistic simulation of fusion materials with LAMMPS and FitSNAP	THOMPSON, Aidan (Sandia National Laboratories)
09:30	Multiscale modeling of diffusion phenomena in nuclear fuels : from the atomic scale to phase-field polycrystalline microstructure evolution simulations	MESSINA, Luca (CEA Cadarache)

## contributed - Press Room (10:00 - 10:20)

time	title	presenter
10:00	Multi-scale modelling of hydrogen isotopes retention and diffusion in highly irradiated materials	KAUR, Sanjeet (United Kingdom Atomic Energy Authority)

## break (10:20 - 11:00)

## invited - Press Room (11:00 - 12:00)

time	title	presenter
11:00	Machine Learned Interatomic Potentials for Extreme Environments	JANSSEN, Jan (Max Planck Institute for Sustainable Materials)
11:30	Towards Advanced Wall Modeling Using Machine Learning and Its Integration with Neutral Transport Simulations	SAITO, Seiki (Yamagata University)

## contributed - Press Room (12:00 - 12:20)

time	title	presenter
12:00	Applying machine learning potential models to the study of hydrogen in metals: accurate property calculations, complex dynamics simulations, and challenges	ODA, Takuji (Seoul National University)

## lunch (12:20 - 13:50)

## invited - Press Room (13:50 - 14:50)

time	title	presenter
13:50	GRACE universal interatomic potential for materials discovery and design	DRAUTZ, Ralf (Ruhr Universitaet Bochum)
14:20	Sensitivity analysis and optimization of multi-scale models for microstructural evolution in metal materials under neutron irradiation	YANG, Zhangcan (Huazhong University of Science and Technology)

## contributed - Press Room (14:50 - 15:10)

time	title	presenter
14:50	Trap-diffusion modelling of diffusion in restricted geometries	VON TOUSSAINT, Udo (Max-Planck-Institute for Plasmaphysics)

## break (15:10 - 15:50)

**invited - Press Room (15:50 - 16:20)**

time	title	presenter
15:50	MD simulations of high-dose irradiation in Tungsten: The Role of Defect Boundary & Morphology	BHARDWAJ, Utkarsh (Bhabha Atomic Research Centre)

**contributed - Press Room (16:20 - 17:00)**

time	title	presenter
16:20	Transport and deuterium interaction with defects in W, EUROFER and W-Cr-Y alloys damaged by heavy ions	OGORODNIKOVA, Olga (National Research Nuclear University "MEPHI" (Moscow Engineering Physics Institute))
16:40	Vacancy dynamics and hydrogen retention in beryllium	MATVEEV, Dmitry (Forschungszentrum Juelich)

**Meeting of the Scientific Committee (closed event) (18:30 - 20:30)**

# Wednesday 28 May 2025

## invited - Press Room (09:00 - 10:30)

time	title	presenter
09:00	Deuterium trapping and release from high-temperature ion irradiated tungsten: experiments and reaction-diffusion simulations	ZIBROV, Mikhail (Max Planck Institute for Plasma Physics)
09:30	Deuterium Retention Behavior in Tungsten After Plasma Exposure at Varying Temperatures	ZHU, Xiu-Li (North China Electric Power University)
10:00	Deuterium effect on defect evolution in tungsten, from bulk to surfaces	GRANBERG, Fredric (University of Helsinki)

## break (10:30 - 11:10)

## invited - Press Room (11:10 - 11:40)

time	title	presenter
11:10	Investigating the Influence of Helium on Screw Dislocation Mobility in Tungsten	NUTTER, Matt (University of Warwick)

## contributed - Press Room (11:40 - 12:20)

time	title	presenter
11:40	Surface Characterization of Advanced Tungsten and Ceramic Plasma-Facing Materials	KOLASINSKI, Robert (Sandia National Laboratories)
12:00	Nanoindentation and Defect Behavior in Irradiated FCC NiFe Alloys: Experimental Insights and Atomistic Modeling	DOMINGUEZ GUTIERREZ, Francisco Javier (National Centre for Nuclear Research)

## Discussion - Press Room (12:20 - 13:00)

## Closing - Press Room (13:00 - 13:10)