

Program

26–28 May 2025

MoD-PMI 2025

IAEA, Press Room
Vienna International Centre Wagramer Strasse 5 1220 Vienna Austria

Monday 26 May

09:15

Welcome

Session | Location: IAEA, Press Room, Vienna International Centre Wagramer Strasse 5 1220 Vienna Austria

09:35

09:35

invited

Session | Location: IAEA, Press Room, Vienna International Centre Wagramer Strasse 5 1220 Vienna Austria

09:35–10:05 **Alternative plasma facing material for nuclear fusion reactors**

Speaker

Raquel GONZALEZ-ARRABAL (Universidad Politécnica de Madrid)

10:05–10:35 **Experiments and modeling of hydrogen isotope inventory in damaged tungsten**

Speaker

Makoto KOBAYASHI (National Institute for Fusion Science)

10:35

10:35

contributed

Session | Location: IAEA, Press Room, Vienna International Centre Wagramer Strasse 5 1220 Vienna Austria

10:35–10:55 **A kinetic model based on DFT for H atoms transport at the W/Cu interface**

Speaker

Yves FERRO (Aix-Marseille University)

10:55

10:55

break

Break | Location:

11:25

11:25

invited

Session | Location: IAEA, Press Room, Vienna International Centre Wagramer Strasse 5 1220 Vienna Austria

11:25–11:55 **A foundation model for atomistic materials chemistry**

Speaker

Gabor CSANYI (University of Cambridge)

11:55–12:25

From Grains to Gigabytes: Generating Massive Virtual Specimens for Irradiation Damage Study

Speaker

Younggak SHIN (Yonsei University)

12:25–12:55 **Point-Defect-Induced Metastable Phase Diagrams**

Speaker

Maylise NASTAR (CEA)

12:55

12:55

contributed

Session | Location: IAEA, Press Room, Vienna International Centre Wagramer Strasse 5 1220 Vienna Austria

12:55–13:15

Microstructure impact on tritium retention and permeation in tungsten/oxide interface from first-principles based phase field modelling

Speaker

Duc NGUYEN-MANH (United Kingdom Atomic Energy Authority)

13:15

13:15

lunch**Break** | **Location:**

14:30

14:30

invited**Session** | **Location:** IAEA, Press Room, Vienna International Centre Wagramer Strasse 5 1220 Vienna Austria

14:30–15:00

Detection of defects in displacement-damaged tungsten and iron**Speaker**

Sabina MARKELJ (Jozef Stefan Institute)

15:00–15:30

Positron Annihilation Spectroscopy for vacancy defects studies in irradiated tungsten: Combination of modelling and experiments for vacancy size distribution and impurities interaction determination**Speaker**

Marie-France BARTHE (CNRS)

15:30

15:30

contributed**Session** | **Location:** IAEA, Press Room, Vienna International Centre Wagramer Strasse 5 1220 Vienna Austria

15:30–15:50

Impact of the trapping model on Tritium retention and permeation in DEMO Tungsten/Eurofer First Wall**Speaker**

Etienne HODILLE (CEA-IRFM, F-13108 Saint Paul Lez Durance, France)

15:50

15:50

break**Break** | **Location:** IAEA, Press Room, Vienna International Centre Wagramer Strasse 5 1220 Vienna Austria

16:20

16:20

invited**Session** | **Location:** IAEA, Press Room, Vienna International Centre Wagramer Strasse 5 1220 Vienna Austria

16:20–16:50

Adsorption and in-diffusion of Hydrogen at metal and metal oxide surfaces**Speaker**

Katsuyuki FUKUTANI (University of Tokyo)

16:50–17:20

Interface-induced enhanced deuterium plasma-driven permeation in chemical vapor deposition tungsten-copper composite**Speaker**

Long CHENG (Beihang University)

17:20

Tuesday 27 May

09:00

invited

Session | Location: IAEA, Press Room, Vienna International Centre Wagramer Strasse 5 1220 Vienna Austria

09:00–09:30

Quantum-accurate large-scale atomistic simulation of fusion materials with LAMMPS and FitSNAP

Speaker

Aidan THOMPSON (Sandia National Laboratories)

09:30–10:00

Multiscale modeling of diffusion phenomena in nuclear fuels: from the atomic scale to phase-field polycrystalline microstructure evolution simulations

Speaker

Luca MESSINA (CEA, DES, IRESNE, DEC, France)

10:00

10:00

contributed

Session | Location: IAEA, Press Room, Vienna International Centre Wagramer Strasse 5 1220 Vienna Austria

10:00–10:20

Multi-scale modelling of hydrogen isotopes retention and diffusion in highly irradiated materials

Speaker

Sanjeet KAUR (United Kingdom Atomic Energy Authority)

10:20

10:20

break

Break | Location:

11:00

11:00

invited

Session | Location: IAEA, Press Room, Vienna International Centre Wagramer Strasse 5 1220 Vienna Austria

11:00–11:30

Machine Learned Interatomic Potentials for Extreme Environments

Speaker

Jan JANSSEN (Max Planck Institute for Sustainable Materials)

11:30–12:00

Towards Advanced Wall Modeling Using Machine Learning and Its Integration with Neutral Transport Simulations

Speaker

Seiki SAITO (Yamagata University)

12:00

12:00

contributed

Session | Location: IAEA, Press Room, Vienna International Centre Wagramer Strasse 5 1220 Vienna Austria

12:00–12:20

Applying machine learning potential models to the study of hydrogen in metals: accurate property calculations, complex dynamics simulations, and challenges

Speaker

Takuji ODA (Seoul National University)

12:20

12:20

lunch

Break | Location:

13:50

13:50

invited

Session | Location: IAEA, Press Room, Vienna International Centre Wagramer Strasse 5 1220 Vienna Austria

13:50–14:20

GRACE universal interatomic potential for materials discovery and design**Speaker**

Ralf DRAUTZ (Ruhr Universitaet Bochum)

14:20–14:50

Sensitivity analysis and optimization of multi-scale models for microstructural evolution in metal materials under neutron irradiation**Speaker**

Zhangcan YANG (Huazhong University of Science and Technology)

14:50

14:50

contributed

Session | Location: IAEA, Press Room, Vienna International Centre Wagramer Strasse 5 1220 Vienna Austria

14:50–15:10

Trap-diffusion modelling of diffusion in restricted geometries**Speaker**

Udo VON TOUSSAINT (Max-Planck-Institute for Plasmaphysics)

15:10

15:10

break

Break | Location:

15:50

15:50

invited

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15:50–16:20

MD simulations of high-dose irradiation in Tungsten: The Role of Defect Boundary & Morphology**Speaker**

Utkarsh BHARDWAJ (Bhabha Atomic Research Centre)

16:20

16:20

contributed

Session | Location: IAEA, Press Room, Vienna International Centre Wagramer Strasse 5 1220 Vienna Austria

16:20–16:40

Transport and deuterium interaction with defects in W, EUROFER and W-Cr-Y alloys damaged by heavy ions**Speaker**

Olga OGORODNIKOVA (National Research Nuclear University "MEPHI" (Moscow Engineering Physics Institute))

16:40–17:00

Vacancy dynamics and hydrogen retention in beryllium**Speaker**

Dmitry MATVEEV (Forschungszentrum Juelich)

17:00

18:30

20:30

Meeting of the Scientific Committee (closed event)

Break | Location:

Wednesday 28 May

09:00

invited

Session | Location: IAEA, Press Room, Vienna International Centre Wagramer Strasse 5 1220 Vienna Austria

09:00–09:30

Deuterium trapping and release from high-temperature ion irradiated tungsten: experiments and reaction-diffusion simulations

Speaker

Mikhail ZIBROV (Max Planck Institute for Plasma Physics)

09:30–10:00

Deuterium Retention Behavior in Tungsten After Plasma Exposure at Varying Temperatures

Speaker

Xiu-Li ZHU (North China Electric Power University)

10:00–10:30

Deuterium effect on defect evolution in tungsten, from bulk to surfaces

Speaker

Fredric GRANBERG (University of Helsinki)

10:30

10:30

break

Break | Location:

11:10

11:10

invited

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11:10–11:40

Investigating the Influence of Helium on Screw Dislocation Mobility in Tungsten

Speaker

Matt NUTTER (University of Warwick)

11:40

11:40

contributed

Session | Location: IAEA, Press Room, Vienna International Centre Wagramer Strasse 5 1220 Vienna Austria

11:40–12:00

Surface Characterization of Advanced Tungsten and Ceramic Plasma-Facing Materials

Speaker

Robert KOLASINSKI (Sandia National Laboratories)

12:00–12:20

Nanoindentation and Defect Behavior in Irradiated FCC NiFe Alloys: Experimental Insights and Atomistic Modeling

Speaker

Francisco Javier DOMINGUEZ GUTIERREZ (National Centre for Nuclear Research)

12:20

12:20

Discussion

Session | Location: IAEA, Press Room, Vienna International Centre Wagramer Strasse 5 1220 Vienna Austria

13:00

13:00

Closing

Session | Location: IAEA, Press Room, Vienna International Centre Wagramer Strasse 5 1220 Vienna Austria

13:10