# **MoD-PMI 2025**

# Monday 26 May 2025

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

| time  | [id] title   | presenter                |
|-------|--|--------------------------|
| 09:35 | [21] Alternative plasma facing material for nuclear fusion reactors    | GONZALEZ-ARRABAL, Raquel |
| 10:05 | [18] Experiments and modeling of hydrogen isotope inventory in damaged | KOBAYASHI, Makoto        |
|       | tungsten   |                          |

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

| time  | [id] title   | presenter         |
|-------|--|-------------------|
| 11:25 | [44] A foundation model for atomistic materials chemistry  | CSANYI, Gabor     |
| 11:55 | [14] From Grains to Gigabytes: Generating Massive Virtual Specimens for Irradiation Damage Study | Dr SHIN, Younggak |
| 12:25 | [39] Point-Defect-Induced Metastable Phase Diagrams  | NASTAR, Maylise   |

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

| time  | e [id] title presenter  |                         |
|-------|---|-------------------------|
| 14:30 | [53] Detection of defects in displacement-damaged tungsten and iron   | MARKELJ, Sabina         |
| 15:00 | [54] Positron Annihilation Spectroscopy for vacancy defects studies in irradiated tungsten: Combination of modelling and experiments for vacancy size distribution and impurities interaction determination | Dr BARTHE, Marie-France |

#### invited - Press Room (16:20 - 17:20)

| time  | [id] title   | presenter           |
|-------|--|---------------------|
| 16:20 | [49] Adsorption and in-diffusion of Hydrogen at metal and metal oxide surfaces   | FUKUTANI, Katsuyuki |
| 16:50 | [3] Interface-induced enhanced deuterium plasma-driven permeation in chemical vapor deposition tungsten-copper composite | CHENG, Long         |

# Tuesday 27 May 2025

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

| time  | [id] title   | presenter       |
|-------|--|-----------------|
| 09:00 | [36] Quantum-accurate large-scale atomistic simulation of fusion materials with LAMMPS and FitSNAP   | THOMPSON, Aidan |
| 09:30 | [60] Multiscale modeling of diffusion phenomena in nuclear fuels : from the atomic scale to phase-field polycristalline microstructure evolution simulations | MESSINA, Luca   |

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

| time  | [id] title   | presenter    |
|-------|--|--------------|
| 11:00 | [58] Machine Learned Interatomic Potentials for Extreme Environments   | JANSSEN, Jan |
| 11:30 | [47] Towards Advanced Wall Modeling Using Machine Learning and Its<br>Integration with Neutral Transport Simulations | SAITO, Seiki |

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

| time  | [id] title   | presenter      |
|-------|--|----------------|
| 13:50 | [59] GRACE universal interatomic potential for materials discovery and design  | DRAUTZ, Ralf   |
| 14:20 | [9] Sensitivity analysis and optimization of multi-scale models for microstructural evolution in metal materials under neutron irradiation | YANG, Zhangcan |

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

| time  | [id] title   | presenter         |
|-------|--|-------------------|
| 15:50 | [8] MD simulations of high-dose irradiation in Tungsten: The Role of Defect<br>Boundary & Morphology | BHARDWAJ, Utkarsh |

# Wednesday 28 May 2025

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

| time  | [id] title  | presenter         |
|-------|---|-------------------|
| 09:00 | [19] Deuterium trapping and release from high-temperature ion irradiated tungsten: experiments and reaction-diffusion simulations | ZIBROV, Mikhail   |
| 09:30 | [11] Deuterium Retention Behavior in Tungsten After Plasma Exposure at<br>Varying Temperatures                                    | ZHU, Xiu-Li       |
| 10:00 | [52] Deuterium effect on defect evolution in tungsten, from bulk to surfaces  | GRANBERG, Fredric |

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

| time  | [id] title  | presenter    |
|-------|---|--------------|
| 11:10 | [48] Investigating the Influence of Helium on Screw Dislocation Mobility in<br>Tungsten | NUTTER, Matt |