Program

Monday 25 May 2015

13:00 – 14:00	Registration
14:00 – 14:15	Opening ***Yves Ferro***

Session 1 - *Molecular Dynamics*

Chair: Charlotte Becquart

14:15 – 14:50	Self-trapping and trap mutation in bulk tungsten: a DFT and Molecular Dynamics investigation (I1) ***Charlotte Becquart***
14:50 – 15:25	New interatomic potentials for studying the behavior of noble gas atoms in tungsten (I2) ***Huiqiu Deng***
Break	
15:50 – 16:25	Tungsten Fuzzy Nanostructure Growth by Molecular Dynamics and Monte Carlo Hybrid Simulation (I3) ***Atsushi M Itoh***
16:25 – 17:00	Modelling of Hydrogen Interactions with Beryllium Surfaces in Fusion Reactor (I4) ***Pavel Vladimirov***

Session 2

17:00 – 18:30	*Poster session*

Tuesday 26 May 2015

Session 3 –*Quantum Effects In Molecular Dynamics*

Chair: Bas Braams

8:40 – 9:15	Modelling and Data Needs for Plasma-Material Interaction in Fusion Devices: Perspective from the IAEA Atomic and Molecular Data Unit (I5) ***Bas Braams***
9:15 – 9:50	Time-*dependent* simulation of electronic stopping from first-principles (I6) ***Jorge J. Kohanoff***
9:50 – 10:25	Quantum nuclei in materials: (when) do we need to worry? (I7) ***Michele Ceriotti***

Coffee break

11:10 – 11:45	Quantum theory of transport and trapping of hydrogen in iron (I8) ***Anthony Paxton***
11:45 – 12:20	Nuclear quantum effects in tritium diffusion in α-iron (I9) ***Toshiyukii Takayanagi***

Lunch

Session 4 – *Experimental Data for Modelling*

Chair: Gregory de Temmerman

14:00 – 14:35	The need for a better understanding of plasma-material interactions in ITER and the role of modelling (I10) ***Gregory de Temmerman***
14:35 – 15:10	Vacancy defects studied in tungsten by using Positron annihilation spectroscopy (I11) ***Marie-France Barthe***
15:10 – 15:45	Experimental studies of hydrogen transport parameters in tungsten (I12) ***Heun-Tae Lee***

Coffee break

16:25 – 16:50	Influence of aluminum oxide coating oxygen presence in plasma on deuterium retention in tungsten (O1) ***Leon Begrambekov***
16:50 – 17:15	Deuterium retention in polycrystalline tungsten at low fluences (O2) ***Régis Bisson***

Summary and discussion

17:15 – 18:00

Wednesday 27 May 2015

Session 5 *– Multi-scale modelling 1: DFT and statistic methods*

Chair: Joerg Neugebauer

8:40 – 9:15	Understanding the fundamental mechanisms behind H embrittlement: An ab initio guided multiscale approach (I13) ***Jörg Neugebauer***
9:15 – 9:50	Setting up plasma pulse-scale simulations with electronic structure calculations (I14) **Kalle *Heinola***
9:50 – 10:25	Hydrogen recycling in tungsten during plasma pulse simulations with rate equations (I15) ***Tommy Ahlgren***

Coffee break

Chair: Daiji Kato

11:05 – 11:40	Multiscale modelling of radiation effects in materials: ion implantation versus neutron irradiation (I16) ***Maria José Caturla Terol***
11:40 – 12:05	Hydrogen trapping at vacanciesand hydrogen impact on vacancy diffusion and self-diffusion in Ni (O3) ***Döme Tanguy***
12:05 – 12:30	Vacancy nanoclusters in irradiated W and W alloys: First-principles assessments and multi-scale modelling (O4) ***Duc Nguyen-Manh***

Lunch

Session 6 *– Multi-scale modelling 2: Rate-equations and Reaction Diffusion models*

Chair: Klaus Schmid

14:00 – 14:35	Modeling isotope exchange in W using fill level dependent trapping (I17) ***Klaus Schmid***
14:35 – 15:10	Macroscopic rate equation modeling of trapping/detrapping of hydrogen isotopes in tungsten materials (I18) ***Christian Grisolia***

Coffee break

15:40 – 16:15	Migration, trapping and release of deuterium from tungsten in the presence of high density of defects: theory and experiment (I19) ***Olga Ogorodnikova***
16:15-16:35	Materials research in Jülich: hydrogen retention in beryllium (O5) ***Dmitry Matveev***

Summary and discussion

16:35- 17:15

Closing