

## PROGRAMME

Lectures, other presentations and computer training are all held in **Room 601, Building No. 4, ASIPP**. The posters are in an adjacent area starting on Tuesday.

### Sunday 17 July 2016 / Arrival

- 14:00 -
- 18:00 Registration (lobby of Best Western Premier Hotel Hefei)

### Monday 18 July 2016 / Day 1

- 07:40 Shuttle bus to ASIPP (main gate of Best Western Premier Hotel Hefei)
- 08:00 -
- 08:30 Registration (entrance of meeting room 601)
- 08:30 -
- 09:00 Opening by Prof. Wan (Director of ASIPP) and Dr. Braams (Chaired by Luo)

#### Session L1 – Lecturer: Linsmeier

- 09:00 -
- 10:20 Lecture 1: Plasma surface interactions
- 10:20 -
- 10:40 Photograph taking and Coffee break
- 10:40 -
- 12:00 Lecture 2: Plasma-facing materials
- 12:00 -
- 13:30 Lunch

#### Session L2 – Lecturer: Luo

- 13:30 -
- 15:00 Lecture 3: Plasma-facing components
- 15:10 -
- 15:30 Coffee break

#### Session O1: Experiments – Chairman: Linsmeier

- 15:30 - I1: Huiqiu Deng, Molecular dynamics simulation of the wetting behaviors of liquid Li on W surface
- 15:55 -
- 15:55 - O1: Petter Ström, Ion beam methods for the study of plasma-facing materials
- 16:10 -
- 16:10 - O2: Yuping Xu, Plasma-Material Interaction experiments during the 2015 spring EAST campaign employing MAPES
- 16:25 -
- 16:25 - O3: Xiu-Li Zhu, Deuterium behavior in argon-damaged tungsten exposed to high flux and low energy deuterium plasma
- 16:40 -
- 16:40 - O4: Younggil Jin, TDS Study of Effect of High Energy Ion induced Cascade Collisional Damage on Deuterium Retention in Tungsten
- 16:55 -
- 16:55 - O5: Long Cheng, Investigation of surface morphology and deuterium retention in tungsten exposed to neon and deuterium mixture plasmas in Pilot-PSI
- 17:10 -
- 17:30 -
- 20:00 Reception

20:00 Shuttle bus to hotel (main gate of 4th building of ASIPP)

## **Tuesday 19 July 2016 / Day 2**

07:40 Shuttle bus to ASIPP (main gate of Best Western Premier Hotel Hefei)

### **Session L3 – Lecturer: Neugebauer**

08:30 – Lecture 4: Ab initio description of defects in materials under extreme conditions (1)  
10:00

10:00 – Coffee break  
10:20

10:20 – Lecture 5: Ab initio description of defects in materials under extreme conditions (2)  
11:50

12:00 – Lunch  
13:30

### **Session O2: Tungsten (1) – Chairman: Neugebauer**

13:30 – I2: Chang-Song Liu, TBD  
13:55

13:55 – O6: XianShan Kong, Towards understanding the differences in irradiation effects of He, Ne and Ar plasma by investigating the physical origin of their clustering in tungsten  
14:10

14:10 – O7: Li-Fang Wang, A new embedded-atom method interatomic potential for tungsten-hydrogen system  
14:25

14:25 – O8: Yinan Wang, Hydrogen-induced change in core structures of screw and edge dislocations in Tungsten  
14:40

14:40 – O9: Jiechao Cui, Estimation of the lifetime of small helium bubbles near tungsten surfaces - a methodological study.  
14:55

14:55 – O10: Jie Hou, Retention behavior of hydrogen isotopes in tungsten revisited by multi-scale modelling  
15:10

15:10 – Coffee break  
15:30

15:30 – Lab tour to ISSP and ASIPP  
18:00

18:00 Shuttle bus to hotel (main gate of 4th building of ASIPP)

## **Wednesday 20 July 2016 / Day 3**

07:40 Shuttle bus to ASIPP (main gate of Best Western Premier Hotel Hefei)

### **Session L4 – Lecturer: Gao and Wirth**

08:30 – Lecture 6 by Gao: Molecular dynamics simulations of fusion materials: challenges and opportunities (1)  
10:00

10:00 – Coffee break  
10:20

10:20 – Lecture 7 by Wirth: Introduction on Xolotl PSI code  
11:50

12:00 – Lunch  
13:30

### **Session O3: Tungsten (2) – Chairman: Gao**

13:30 – O11: Yu-Wei You, Clustering of transmutation solutes Re, Os, and Ta and its influence on helium bubble formation in tungsten  
13:45

13:45 – O12: Jingzhong Fang, Molecular dynamics simulations of the clustering and

- 14:00 dislocation loop punching behaviors of noble gas atom in tungsten
- 14:00 – O13: Zhancan Yang, Kinetic Monte Carlo Simulations of Helium Cluster
- 14:15 Nucleation in Tungsten with Pre-Existing Vacancies
- 14:15 – O14: Haohua Wen, Interpretation of non-Arrhenius diffusion of helium in BCC
- 14:30 Tungsten
- 14:30 – O15: Yulu Zhou, Monte Carlo simulations of helium bubble growth and gas release
- 14:45 in tungsten
- 14:45 – Coffee break
- 15:00

#### **Session CT**

- 15:00 – Training on Xolotl by Prof. Wirth
- 16:30
- 16:30 – Training on LAMMPS by Prof. Gao
- 18:00
- 18:00 Shuttle bus to hotel (main gate of 4th building of ASIPP)

#### **Thursday 21 July 2016 / Day 4**

- 07:40 Shuttle bus to ASIPP (main gate of Best Western Premier Hotel Hefei)

#### **Session L5 – Lecturer: Wirth and Gao**

- 08:30 – Lecture 8 by Wirth: Atomistic modeling of helium diffusion and clustering behavior
- 10:00 in tungsten
- 10:00 – Coffee break
- 10:20
- 10:20 – Lecture 9 by Gao: Molecular dynamics simulations of fusion materials: challenges
- 11:50 and opportunities (2)
- 12:00 – Lunch
- 13:30

#### **Session O4: Iron – Chairman: Wirth**

- 13:30 – I3: Qing HOU, TBD
- 13:55
- 13:55 – O16: Jingyi Shi, Atomistic study on the growth of helium bubbles in  $\alpha$ -Fe from the
- 14:10 view of energetics and mechanics
- 14:10 – O17: Tao Lu, Atomistic study of hydrogen behavior around a screw dislocation in
- 14:25 alpha iron
- 14:25 – O18: Jianhua Ding, The magnetism (Fe, Cr, and the stability of He-vacancy
- 14:40 complexes in Fe-9Cr alloys
- 14:40 – O19: Yange Zhang, Effect of carbon and alloying solute atoms on helium behaviors
- 14:55 in  $\alpha$ -Fe
- 14:55 – O20: Amit Sharma, Adaptive Kinetic Monte Carlo Study of Hydrocarbon
- 15:10 Diffusion/Trapping in First-Wall and Amorphous Hydrocarbon Flakes
- 15:10 – Coffee break
- 15:30

#### **Session P**

- 15:30 – Poster session (Starting from Tuesday)
- 18:00
- 18:00 Shuttle bus to hotel (main gate of 4th building of ASIPP)

**Friday 22 July 2016 / Day 5**

07:40 Shuttle bus to ASIPP (main gate of Best Western Premier Hotel Hefei)

**Session L6 – Lecturer: Lu**

08:30 – Lecture 10: Introduction to first-principles method  
10:00 –  
10:00 – Coffee break  
10:20 –  
10:20 – Lecture 11: Applications of first-principles method in studying fusion materials  
11:50 –  
12:00 – Lunch  
13:30 –

**Session O5: Damages – Chairman: Lu**

13:30 – I4: Jizhong Sun, Deuterium bubble bursting in tungsten  
13:55 –  
13:55 – O21: P. N. Maya, Simulation Studies on Radiation Induced Defects and Stress in  
14:10 Tungsten  
14:10 – O22: Baoqin Fu, Molecular Dynamics Study of the Dislocation Effect on  
14:25 displacement cascade in Tungsten  
14:25 – O23: Yuexia Wang, Mechanical response of Ti<sub>3</sub>SiC<sub>2</sub> to He/H irradiation:  
14:40 Elaboration from first-principles calculation  
14:40 – O24: Xuebang Wu, Influence of alloying additions on grain boundary cohesion in  
14:55 tungsten: First-principles predictions and opportunities  
14:55 – O25: Yonggang Li, Ion radiation albedo effect: influence of surface roughness on  
15:10 ion retention and sputtering of materials  
15:10 –  
15:10 – Coffee break  
15:30 –

**Session R: Review and Closing**

15:30 – Discussion chaired by Braams  
16:30 –  
16:30 – Summary by Luo and Closing by Braams  
17:00 –  
17:00 Shuttle bus to hotel (main gate of 4th building of ASIPP)

**Saturday 23 July 2016 / Departure**