

**Workshop on
Modeling the property of engineering
materials and its applications
MPEMA-I**

Host Units: Chongqing University

Royal Institute of Technology

Chongqing, China

May 22-25, 2018

Tuesday 22nd of May 2018

Registration and Visiting

Wednesday 23rd of May 2018

9:00 Opening: Dengfu Chen

Chairperson: **Jian Sun**

9:20	Levente Vitos	Introduction of AMP group at KTH
9:40	Dengfu Chen/ Huamei Duan	Intoduction of 2M group at CQU
10:00	Se Kyun Kwon	Twinnability in fcc metals and alloys
10:25	Qingmiao Hu	First-principles investigations of the microstructure and mechanical properties of titanium alloys
10:50	Mujun Long	In-situ observation of second phase particles and austenite grain growth in Ti microalloyed steel
11:15	Jianhong Dai	First principles study on the oxidation properties of titanium alloys

11:40-14:00 Lunch

Chairperson: **Se Kyun Kwon**

14:00	Jian Sun	A First-principles Study of Displacive Phase Transitions and Mechanical Twinning in β Ti-V alloys
14:25	Narisu	Lattice dynamics of FeMnP0.5Si0.5 compound from first principles calculation
14:50	Raquel Lizarraga	High entropy alloys: substituting for Co in cutting-edge technology
15:15	Liyun Tian	Ab initio descriptions of short-range order in random Cu-Au alloys
15:35	Ruiwen Xie	Constructing an equation to calculate COM values with an ab-initio method - EMTO

15:55-16:15 *Coffee*

Chairperson: Qingmiao Hu

16:15	Guisheng Wang	The unstable stacking fault energies of transition metals
16:40	Wei Li	To be defined
17:00	Wenxiang Jiang	Research Progress on High Temperature Properties of Continuous Casting Slab
17:20	Xun Sun	Elastic properties of $Al_xCrMnFeCoNi$ ($0 \leq x \leq 5$) high-entropy alloys from ab initio theory
17:40	Sheng Yu	Fluid Flow and Solidified Shell Re-melting in the F-EMS Area during Billet Continuous Casting

Evening program

Thursday 24th of May 2018

Chairperson: **Qingcai Liu**

9:30-11:30	Levente Vitos	Plasticity of austenitic steels from quantum mechanical modeling (<i>presentation at college level</i>)
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11:30-14:00 *Lunch*

Chairperson: **Mujun Long**

14:00	Hualei Zhang	Phase selection rule for Al-doped CrMnFeCoNi high-entropy alloys from first-principles
14:25	Wenyue Zhao	First-principles prediction of the thermo-mechanical properties of Ni-Mo solid solution in Ni-based superalloys
14:50	Linggang Zhu	Structure prediction of the transition metal oxides
15:15	Song Lu	First-principles study of heterophase interface
15:35	Henrik Lev äm äki	An automated algorithm for reliable equation of state fitting of magnetig systems

15:55-16:15 *Coffee*

Chairperson: **HuaLei Zhang**

16:15	Young Won Choi	First Principles Study on the Embrittlement of Fe-Si Alloys
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16:35	Xiaojie Li	Understanding the mechanical properties of reduced activation steels
16:55	D ávid Moln á	Relationship between mechanical behavior and stacking fault energy in austenitic stainless steels
17:15	Shuo Huang	Mapping the magnetic transition temperatures for medium- and high-entropy alloys
17:35	Zhihua Dong	Plastic deformation modes in paramagnetic γ -Fe from longitudinal spin fluctuation theory

17:55 Closing: Levente Vitos

Evening program

Friday 25th of May 2018

9:30-11:30 Laboratory Visiting

Contacts:

Huamei Duan (段华美), Chongqing University, +86 15002311931,
duanhuamei@cqu.edu.cn

Dengfu Chen (陈登福), Chongqing University, +86 13658333267,
chendfu@cqu.edu.cn

Mujun Long (龙木军), Chongqing University, +86 13594318151,
longmujun@cqu.edu.cn

Tel: +86 23 65102467