Session Program

13–17 Sept 2021

EUROPEAN CONGRESS AND EXHIBITION ON ADVANCED MATERIALS AND PROCESSES - EUROMAT 2021

D6_Atomic scale modelling of advanced materials - Ab initio, molecular dynamics and Monte-Carlo simulations

Virtual

Wednesday 15 September

09:50

D6_Atomic scale modelling of advanced materials - Ab initio, molecular dynamics and Monte-Carlo simulations: D6_1_Machine learning techniques for atomistic simulations I

Session | **Location:** Room 12

09:50–10:30

Atomic cluster expansion for accurate and transferable interatomic potentials (Keynote)

Speaker
Prof. Ralf Drautz

10:30–10:50

Automated parameterization of the Atomic Cluster Expansion

Speaker
Dr Anton Bochkarev

10:50–11:10

Geometrical descriptors for predicting kinetic barriers in battery cathode materials

Speaker
Felix Tim Bölle

11:10–11:30

Prismatic slip in pure Magnesium with a Neural Network Potential

Speaker
Prof. Markus Stricker

11:30

11:50

D6_Atomic scale modelling of advanced materials - Ab initio, molecular dynamics and Monte-Carlo simulations: D6_2_Electronic Structure and Transport

Session | **Location:** Room 12

11:50–12:10

Machine learned force fields: status and challenges (Highlight)

Speaker
Gabor Csanyi

12:10–12:30

Identifying the bottlenecks for heat transport in metal-organic frameworks (Highlight)

Speaker
Sandro Wieser

12:30–12:50

Mixed Metal Oxides - Tracking Oxidation States using DFT

Speaker
Alexander Genest

12:50–13:10

Electronic and optical properties of quaternary chalcogenide solid solutions

Speaker
Dr Daniel Fritsch

13:10

15:30

D6_Atomic scale modelling of advanced materials - Ab initio, molecular dynamics and Monte-Carlo simulations: D6_3_Thermodynamics

Session | **Location:** Room 12

15:30–15:50 **Development of an ab initio free energy database (Highlight)**

Speaker
Blazej Grabowski

15:50–16:10

Accurate prediction of random alloy equilibrium properties based on the coherent potential approximation

Speaker
Mr Franco Moitzi

16:10–16:30

Accurate on-lattice model for investigation kinetics of precipitates formation in multicomponent systems

Speaker
Evgenii Meshkov

16:30–16:50 **Automated calculation of phase diagrams from interatomic potentials**

Speaker
Mr Sarath Menon

16:50–17:10

Crystal chemistry of novel binary Ag-Cl phases from ab initio: from simple ionic compounds to clustered compounds and silver polychlorides.

Speaker
Dr Mariana Derzsi

17:10

Thursday 16 September

09:50

D6_Atomic scale modelling of advanced materials - Ab initio, molecular dynamics and Monte-Carlo simulations: D6_4_Hydrogen

Session | **Location:** Room 12

09:50–10:10 **Hydrogen effect on vacancy diffusion in metals (Highlight)**

Speaker
Prof. Shigenobu Ogata

10:10–10:30

Atomistic study of hydrogen behavior in Fe in presence of crystal defects

Speaker
Dr Sergei Starikov

10:30–10:50

Ab Initio Study of Hydrogen Solution and Embrittlement at Cleavage Planes and Grain Boundaries in Bcc Iron

Speaker
Abril Azocar Guzman

10:50

11:50

D6_Atomic scale modelling of advanced materials - Ab initio, molecular dynamics and Monte-Carlo simulations: D6_5_Mechanical properties - Grain boundaries

Session | **Location:** Room 12

11:50–12:10

Inversion boundary formation in doped ZnO investigated from first principles

Speaker
Dr Jürgen Spitaler

12:10–12:30

First-principles study of solute grain boundary interactions in a BCC Ti-Mo alloy

Speaker
Mr Hariharan Umashankar

12:30–12:50

Segregation of Cr, Cu, Mn, Mo, Ni and P to bcc-Fe GBs and their effects on grain boundary cohesion: a first principles study

Speaker
Mr Han Mai

12:50–13:10 **Influence of segregation on the adhesion of the Cu-WTi Interface**

Speaker
Mr Rishi Bodlos

13:10–13:30

Modelling interactions between kinetics of grain boundary segregation and precipitation

Speaker
Dr Daniel Scheiber

13:30

14:40

D6_Atomic scale modelling of advanced materials - Ab initio, molecular dynamics and Monte-Carlo simulations: D6_6_Point defects

Session | **Location:** Room 12

14:40–15:00
Machine learning of segregation energies obtained with atomistic simulations

Speaker
Prof. Lorenz Romaner

15:00–15:20
Multi-Scale Modelling of the Clustering Processes and Mobility Properties of Vacancies in Cu

Speaker
Mr Vasileios Fotopoulos

15:20–15:40
Vacancy properties in the Nb-Ti-Zr bcc system from ab initio simulations

Speaker
Mrs Sally Issa

15:40–16:00
Generative model of defects produced by displacement cascades in Zr

Speaker
Dr Bartosz Barzdajn

16:00–16:20
Ab initio prediction of vacancy formation and migration properties in HCP high entropy alloys

Speaker
Dr Xi Zhang

16:20

16:40

D6_Atomic scale modelling of advanced materials - Ab initio, molecular dynamics and Monte-Carlo simulations: D6_7_Mechanical properties - elasticity, plasticity

Session | **Location:** Room 12

16:40–17:00
Two-scale simulation of plastic deformation in bcc metals: combination of atomistic simulation and dislocation dynamics

Speaker
Dr Sergei Starikov

17:00–17:20 **Investigation of tungsten plasticity using atomic cluster expansion**

Speaker
Antoine Kraych

17:20–17:40
Dynamical and mechanical properties of single AgF2 nanowire from ab initio

Speaker
Dr Kamil Tokar

17:40–18:00

Solute drag assessment of grain boundary migration in Au using atomistic simulations

Speaker
Mr Ayush Suhane

18:00–18:20

Understanding the Anisotropic Elastic Properties of Metal-Organic Frameworks: The Instructive Example of MOF-74

Speaker
Mr Tomas Kamencek

18:20

Friday 17 September

09:50

D6_Atomic scale modelling of advanced materials - Ab initio, molecular dynamics and Monte-Carlo simulations: D6_8_Magnetism

Session | **Location:** Room 12

09:50–10:30

Spin-orbit coupling: a never-ending source for complex magnetism (Keynote)

Speaker
Dr Silvia Picozzi

10:30–10:50

Strong Magnetism in Strongly-Correlated Electronic Systems from an Ab-initio Perspective (Highlight)

Speaker
Dr Markus Aichhorn

10:50–11:10

Stoner ferromagnetism in 2D aluminum nitrides

Speaker
Mr Ruishen Meng

11:10–11:30

On using an auxiliary magnetic charge density to calculate the magnetostatic dipole-dipole correction to spin-density functional theory (DFT)

Speaker
Lórien MacEnulty

11:30

11:50

D6_Atomic scale modelling of advanced materials - Ab initio, molecular dynamics and Monte-Carlo simulations: D6_9_Complex methodologies I

Session | **Location:** Room 12

11:50–12:10

Watching polymer networks form: Molecular dynamics simulation of the chain growth polymerization of photopolymers

Speaker
Alexander Hochwallner

12:10–12:30

High-throughput calculations for the search of magnetocaloric materials

Speaker
Mr Rafael Vieira

12:30–12:50

Systematic Coarse-Graining in Metal-Organic Frameworks

Speaker
Mr Sander Vandenhaute

12:50–13:10

First-principles study of Graphene-Au clusters interactions

Speaker
Mr Ramasamy Murugesan

13:10–13:30 **Modelling dynamics of molecules on surfaces**

Speaker
Dr Ivor Loncaric

13:30

14:40

D6_Atomic scale modelling of advanced materials - Ab initio, molecular dynamics and Monte-Carlo simulations: D6_10_Complex methologies II

Session | **Location:** Room 12

14:40–15:00

First-principles studies of (Ru-)doped titanium dioxide clusters as catalysts for photocatalytic ammonia production

Speaker
Taja Žibert

15:00–15:20

A Molecular Model for Hydrated Silicate Ionic Liquids: Towards a Beter Understanding of Zeolite Formation

Speaker
Dr Jelle Vekeman

15:20–15:40

Ab-initio calculation of the temperature-dependent antiphase boundary energy in Ni3Al

Speaker
Xiang Xu

15:40–16:00

Unraveling surface interactions between clathrates and hydrophobic surfaces

Speaker
Dr Paulo Mileo

16:00–16:20

Atomistic Study of Star-shaped Polystyrene and Poly(ethylene-oxide) Melts Through Molecular Dynamics Simulations

Speaker
Mrs Eirini Gkolfi

16:20