

Session Program

13-17 Sept 2021

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

***B8_Theory-guided development structural
materials***

Virtual

Thursday 16 September

16:40

B8_Theory-guided development structural materials: B8_1_Electronic Materials

Session | **Location:** Room 5

16:40-17:20

Doped skyrmionic B20 compounds: magnetic properties and structural stability (Keynote)

Speaker

Dr Vladislav Borisov

17:20-17:40

Impact of magnetochemical interplay on phase stability, defects and diffusion in fcc Fe-Ni alloys

Speaker

Mr Kangming Li

17:40-18:00

Molecular simulation guided synthesis of modified MIL-101(Cr) for selective recovery and separation of rare earth elements

Speaker

Fatemeh Keshavarz

18:00-18:20

High-throughput and Data-mining Search for Rare-earth-free Permanent Magnets

Speaker

Dr Alena Vishina

18:20

Friday 17 September

09:50

B8_Theory-guided development structural materials: B8_2_Atomic Design of structural alloys I

Session | Location: Room 5

09:50–10:10

Modeling polaron hopping in ternary spinel oxides (Highlight)

Speaker

Maytal Caspary Toroker

10:10–10:30

Structural phase stability, mechanical properties and elastic anisotropy of TiAl+Mo alloys: an abinitio assessment

Speaker

Mrs Neda Abdoshahi

10:30–10:50

Investigation of the fcc→bcc phase transformation in a binary system

Speaker

Dr Gilles Demange

10:50

11:50

B8_Theory-guided development structural materials: B8_3_Atomic Design of structural alloys II

Session | Location: Room 5

11:50–12:30

Atomistic Modelling of Low Temperature Precipitation of Iron Carbides in Martensitic Steels (Keynote)

Speaker

Dr Felix Schwab

12:30–12:50

Multi-Scale Atomistic Modelling of Point Defects in Cu Grain Boundaries and Triple Junctions

Speaker

Mr Vasileios Fotopoulos

12:50–13:10

Investigation of phase boundaries using an multiscale atomistic QM/MM approach

Speaker

Dominik Gehringer

13:10

14:40

B8_Theory-guided development structural materials: B8_4_Multi-component alloys

Session | Location: Room 5

14:40–15:00

Predicting phase stability in high entropy TiAl alloys from first principles

Speaker

Mr Lukas Hatzenbichler

15:00–15:40

Machine learning assisted ab initio thermodynamics: from BCC unaries to HEAs (Keynote)**Speaker**

Dr Prashanth Srinivasan

15:40–16:00

Stabilities and mechanical properties of novel Mg-based light metal multi-principal alloys**Speaker**

Dr Wernfried Mayr-Schmölzer

16:00

16:40

B8_Theory-guided development structural materials: B8_5_Functional coatings**Session** | **Location:** Room 5

16:40–17:00

Phase field crystal simulation of the structure transformation from cubic to hexagonal phase and its verification in TiAlN coating**Speaker**

Dr Yi Kong

17:00–17:20

Maximum achievable N content in amorphous nitrides**Speaker**

Dr Jiri Houska

17:20–17:40

Characteristics of Hf(M)SiBCN (M = Y, Ho, Ta, Mo) materials: role of the M choice**Speaker**

Mr Martin Matas

17:40