Theory of Complex Disorder in Materials (TCDM2019)

Monday

10:00 – 10:10 - Opening and welcome

10:10 – 10:50

Active learning of interatomic potentials, **A Shapeev.**

10:50 – 11:10 - Break -

11:10 – 11:30

Phase stability of dynamically disordered solids from first principles, **S I Simak.**

11:30 – 11:40 - Break -

11:40 – 12:00

Accelerating ab-initio studies of alloys properties with active learning of interatomic potentials, **K Gubaev.**

12:00 – 12:10 - Break -

12:10 – 13:40 - Lunch -

13:40 – 14:00

Data-guided approach for multi-principal element alloys discovery, **Y Lysogorskiy.**

14:00 – 14:10 - Break -

14:10 – 14:30

Using machine-learning potentials for vibrational free energy calculations of multicomponent alloys, **P Srinivasan.**

14:30 – 14:40 - Break -

14:40 – 15:00

Dynamic disorder, anharmonicity and phase transformations in perovskite-structured materials from first-principles, **J Klarbring.**

15:30 – 16:10

[Talk title to be announced], **S Biermann.**

16:10 – 16:30 - Break -

16:30 – 17:10

High temperature magnetism and phase stability of 3-d metal and their alloys from DFT-based modeling, **A Ruban.**

17:10 – 17:30 - Break -

17:30 – 17:50

Tuning stacking-fault energies and local lattice distortions in high-entropy alloys, **Y Ikeda.**

17:50 – 18:00 - Break -

18:00 – 21:00 - Poster session with snacks -

21:00 - End -

Tuesday

10:00 – 10:40

Description of Paramagnetism, gap formation and atomic displacements in 3d oxide perovskites in polymorphous DFT, **A Zunger.**

10:40 – 11:00 - Break -

11:00 – 11:40

Electronic Structure and Lattice Stability of Correlated Oxides under High Pressure, **I Leonov.**

11:40 – 12:00 - Break -

12:00 – 12:20

Combined Atomistic Spin Dynamics and Ab Initio Molecular Dynamics: revelation of dynamic spin-lattice coupling in paramgnetic CrN, **B Alling.**

12:20 – 12:30 - Break -

12:30 – 14:00 - Lunch -

14:00 – 14:40

A DMFT insight into the Earth's core: electronic correlations in iron under extreme conditions, **L V Pourovskii.**

14:40 – 15:00 - Break -

15:00 – 15:20

Study of the interplay between magnetic and vibrational degrees of freedom in bcc Fe from first principles, **D Gambino.**

15:20 – 15:30 - Break -

15:30 – 15:50

Impact of magnetic excitations on the energetics of point and extended defects in Fe-Mn alloys, **O Hegde.**

15:50 – 16:00 - Break -

16:00 – 16:20

Magnetic ordering in high entropy alloys: A combined theoretical and experimental study, **B Dutta.**

16:20 – 16:30 - Break -

16:30 – 16:50

Correlated electronic structure with uncorrelated disorder, **A Östlin.**

16:50 – 17:00 - Break -

17:00 – 17:20

Impact of Mo and disorder on diffusion-less transformations in TiAl intermetallic alloys, **D Holec.**

17:20 – 17:30 - Break -

17:30 – 19:00 - Poster session -

19:00 – 20:30 - Dinner -

20:30 - End -

Wednesday

10:00 - 10:40

Lattice Green function calculations in presence of a dislocation, **D R Trinkle.**

10:40 - 11:00 - Break -

11:00 - 11:20

Influence of configurational and magnetic disorder on Screw dislocations from first principle calculations, **L Casillas.**

11:20 - 11:40 - Break -

11:40 - 12:00

Controlling metastable phases of novel nitrides and oxides: from discoveries at extreme conditions towards advanced technological applications, **I A Abrikosov.**

12:00 - 12:10 - Break -

12:10 - 13:40 - Lunch -

13:40 - 14:00

Superionic-like diffusion in an elemental crystal: bcc Titanium, **D G Sangiovanni.**

14:00 - 14:10 - Break -

14:10 - 14:30

icet – A Python library for constructing and sampling alloy cluster expansions, **M Ångqvist.**

14:30 - 14:40 - Break -

14:40 - End -