New Mathematics for the Exascale: Applications to Materials Science

Tuesday March 21, 2023

2:30–3:00 **Michael Taylor** (Los Alamos National Laboratory)
Architector: workflows for rapid generation of sane f-block molecular

3:00–3:30 *Tea Time*

3:30–4:00 **Han Lin Mai** (Max-Planck-Institut für Eisenforschung GmbH)
Cosegregation matters in grain boundary segregation

Thursday March 23, 2023

2:30–3:00 **Maciej Buze** (Heriot-Watt University)
30pmExploring atomistic energy landscapes through bifurcation theory, numerical continuation and deflation techniques

3:00–3:30 *Tea Time*

3:30–4:00 **Andrew Rohskopf** (Sandia National Laboratories)
Exploring model complexity in machine learned potentials with FitSNAP

Tuesday April 4, 2023

2:30–3:00 **Weiqi Chu** (University of California, Los Angeles (UCLA))
A reduced-order method for electron transport with long-range interactions

3:00–3:30 *Tea Time*

3:30–4:00 **Soumendu Bagchi** (Los Alamos National Laboratory)
Atomistic coupling of multiple physical and computational scales in materials plasticity

Thursday April 6, 2023

2:30–3:00 **Thomas Hudson** (University of Warwick)
Mobilities for thermal screw dislocation motion via Large Deviations theory

3:00–3:30 *Tea Time*

3:30–4:00 **Peter Hatton** (Los Alamos National Laboratory)
Long Time-scale Molecular Dynamics Modeling of He Bubble Growth at W Grain Boundaries

Tuesday April 11, 2023

2:30–3:00 **Mira Todorova** (Max-Planck-Institut für Eisenforschung GmbH)
Modelling electrochemical solid/liquid interfaces from first principles

3:00–3:30 *Tea Time*

3:30–4:00 **Jason Gibson** (Los Alamos National Laboratory)
How to ask machine learning models the right questions for material discovery

Thursday April 13, 2023

2:30–3:00
TBA

3:00–3:30 *Tea Time*

3:30–4:00 **Petr Grigorev** (Aix-Marseille University)
Virtual Talk: TBA

Tuesday April 25, 2023

3:00–3:30 *Tea Time*

3:30–4:00 **Jason Gibson** (Los Alamos National Laboratory)
How to ask machine learning models the right questions for material discovery

Thursday April 27, 2023

2:30–3:00 **Maciej Buze** (Heriot-Watt University)
Artificial microstructures: Efficient generation of curved grains with given volumes and aspect ratio

3:00–3:30 *Tea Time*

3:30–4:00
TBA

Tuesday May 9, 2023

2:30–3:00 **Daniel Utt** (OVITO GmbH)
Mapping atoms to a perfect crystal lattice: How to identify dislocations

3:00–3:30 *Tea Time*

3:30–4:00
TBA

Thursday May 11, 2023

2:30–3:00
TBA

3:00–3:30 *Tea Time*

3:30–4:00
TBA

Tuesday May 16, 2023

2:30–3:00 **Elin Theilen** (Fraunhofer MEVIS: Institute for Digital Medicine)
On digital medicine in orthopedic interventions

3:00–3:30 *Tea Time*

3:30–4:00 **Wei Zhu** (University of Alabama)
Variational models in image processing

Thursday May 18, 2023

2:30–3:00
TBA

3:00–3:30 *Tea Time*

3:30–4:00
TBA

Tuesday May 30, 2023

3:00–3:30 *Tea Time*

3:30–4:00
TBA

Thursday June 1, 2023

2:30–3:00
TBA

3:00–3:30 *Tea Time*

3:30–4:00
TBA

Tuesday June 6, 2023

2:30–3:00
TBA

3:00–3:30 *Tea Time*

3:30–4:00
TBA

Thursday June 8, 2023

2:30–3:00 **Eva Zaat** (University of Warwick)
Mathematical modelling of three point bending using asymptotics

3:00–3:30 *Tea Time*

3:30–4:00
TBA