



HPC4EnergyInnovation Special Event

HPC4EI Virtual Event: Focus on Materials

April 8, 2022

8:00 a.m. PDT (11:00 a.m. EDT)

Agenda

8:00 a.m. PDT
(11:00 a.m. EDT)

Welcome

Robin Miles, HPC4EI Program Director, Lawrence Livermore National Laboratory

8:10 a.m. PDT
(11:10 a.m. EDT)

HPC4EnergyInnovation Program Overview: National Laboratories Partner with U.S. Manufacturers to Increase Innovation and Energy Efficiency

Aaron Fisher, HPC4EI Project Manager, Lawrence Livermore National Laboratory

Keynote Speakers

8:30 a.m. PDT
(11:30 p.m. EDT)

Atomistic Modeling and AI for Energy Storage and Conversion

Dr. Rajeev S. Assary, Molecular Materials Group Leader, Argonne National Laboratory

9:15 a.m. PDT
(12:15 p.m. EDT)

Closing the Design Cycle, Image Processing for As-Built Process Simulations

Dr. Scott Roberts, Distinguished R&D Chemical Engineer, Sandia National Laboratories

10:00 a.m. PDT
(1:00 p.m. EDT)

Multiscale Modeling of Catalyst Materials for Carbon Conversion

Dr. Sneha Akhade, Staff Scientist Materials Sciences Division, Lawrence Livermore National Laboratory

10:45 a.m. PDT
(1:45 p.m. EDT)

Break



HPC4EI Projects Featuring Materials Design

11:00 a.m. PDT
(2:00 p.m. EDT)

Phase-Field Simulations of Direct Aging of AM-Processed 718 Alloy

Balasubramaniam Radhakrishnan, Distinguished Research Staff, Oak Ridge National Laboratory

11:20 p.m. PDT
(2:20 p.m. EDT)

Modeling the Antiphase Boundary Energy in Ni₃Al-based Alloys using Density Functional Theory and Machine Learning

Timofey Frolov, Staff Scientist, Lawrence Livermore National Laboratory

11:40 a.m. PDT
(2:40 p.m. EDT)

Accelerating High Temperature Operation Development of High Entropy Alloys via High Performance Computation

Michael Gao, Physical Scientist, National Energy Technology Laboratory

12:00 p.m. PDT
(3:00 p.m. EDT)

***Ab-initio* Guided Design and Materials Informatics for Accelerated Product Development of Next Generation Advanced High Strength Steels**

Sylvie Aubry, Reaction Sorption and Transport Team Lead, Lawrence Livermore National Laboratory

12:20 p.m. PDT
(3:20 p.m. EDT)

Why does material qualification take so long and how can microstructural modeling help?

Mark Messner, Principal Mechanical Engineer, Argonne National Laboratory

12:40 p.m. PDT
(3:40 p.m. EDT)

Closing Remarks

12:45 p.m. PDT
(3:45 p.m. EDT)

Adjourn