S7-1 Advancements in computational, theoretical, and artificial intelligence methods for the accelerated development of ceramics and glassy materials

SHORT DESCRIPTION:

This symposium provides a platform for facilitating knowledge exchange, encouraging collaboration, and addressing the challenges and opportunities in the rapidly evolving fields of atomistic to multiscale simulations, materials informatics, and high-throughput materials design of ceramics and glasses. It welcomes contributions that combine theoretical modeling with experimental/analytical approaches to achieve high-throughput materials design for disorder/amorphous systems. Furthermore, the integration of large language models into simulations and materials informatics will be welcome, highlighting their potential to enhance performance and provide new avenues for designing materials, as well as analyzing and interpreting experimental and theoretical results.

SESSION TOPICS:

• Ab initio, classical, and machine-learning-based atomistic simulations for investigating microstructures and properties of ceramics and glasses.
• Descriptor based thermodynamics for disordered systems.
• Mesoscale, multiscale simulations for overcoming time and length-scales in simulating materials.
• Developing machine-learning and classical force fields.
• Informatics and machine learning technologies for prediction of materials properties and qualities.
• Large language models to enhance performances of simulations and materials informatics.
• High-throughput materials design technologies combining experiments, informatics, simulations, and/or LLMs.

ORGANIZERS:

Stefano Curtarolo, Duke University, USA
Nina Obradović, Institute of Technical Sciences of the Serbian Academy of Sciences and Arts, Serbia
Hiori Kino, The Institute of Statistical Mathematics, Japan
Federica Lodesani, AGC Inc., Italy
Shingo Urata, AGC Inc., Japan