

Recent progress in computational materials science has significantly enhanced the efficiency with which the understanding of fundamental phenomena, the improvement of materials performance, the discovery of new materials, and the design of structural and functional components can be achieved. This symposium will focus on the design and modeling of ceramics and composites with tailored properties so as to further optimize their behavior. A broader perspective is desired that includes the interests related to the ceramic genome, design for new innovative phases and components, integrated computational engineering, prediction of the structure and properties of crystals and defects, modeling materials behavior under extreme/harsh environments, application of novel simulation methods for materials processing and performance, and simulation of ceramics for energy and environmental applications.

Proposed Session Topics:

- Ceramic genome
- Computational engineering of integrated materials
- Multi-scale modeling approaches
- Modeling and design of ceramics for energy and environmental applications
- Modeling materials behavior under extreme/harsh environments (ultrahigh temperature, radiation, environmental damages and severe load and stresses)
- Prediction of the crystal structure and properties of new ceramics
- Modeling defects and amorphous matter

Tentative Organizers:

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