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149th Annual Meeting & Exhibition

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Energy & Environment

Computational Materials Science and Engineering of Materials in Nuclear Reactors

This symposium will focus on the current computational materials science and engineering efforts towards understanding the materials behaviors and microstructure evolutions in nuclear reactors. High neutron flux, thermal and chemical gradients, and corrosive environments cause significant degradation in the microstructural and mechanical properties of materials. Enhanced radiation resistance of structural materials, nuclear fuels, cladding materials and armor materials for plasma facing components are needed to overcome technological challenges necessary for future nuclear systems such as Generation IV fission and fusion reactors.

This symposium seeks abstracts that apply electronic, atomistic, mesoscale and multiscale simulations to discover, understand, and engineer the macroscale performance of fission/fusion reactor materials. This symposium will also consider multiscale modeling efforts that bridge length and time scales in order to better connect simulation results with experimental data for predictive model validation. It will also highlight validation of all relevant models, as well as uncertainty quantification. New computational methods including machine learning approaches, to predict materials behaviors and develop new interatomic potentials for molecular dynamics simulations are also included. Finally, the application of ICME approaches to use modeling and simulation to better understand structure-property relationships, their associated links with performance, and their application to designing future reactor concepts and materials is also desired.

Some examples include:

- Modeling and simulation of materials behavior under extreme environments – radiation, corrosion, stress and temperature, including radiation effects, phase stability, fuel-clad interactions, fission product behavior.
- Developing improved material models for LWR fuel and cladding.
- Modeling and Simulation of TRISO fuel
- Modelling and simulation of radiation damage and their interaction with plasma components in plasma facing materials
- Modeling and simulation of new fuel materials including metal, silicide, and nitride fuels
- New methods to develop interatomic potentials for molecular dynamics simulations
- Modeling and simulation of new cladding materials, such as advanced carbides, coated zirconium alloys, or FeCrAl
- Development and integration of computational tools, methods, and databases for reactor structural material design
- Uncertainty quantification and validation of all the applications listed above

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Abstract Deadline is July 1, 2019. Submit online at
www.programmaster.org/TMS2020.

Questions?
Contact programming@tms.org