

Submission Deadline—July 1, 2017



Architected Materials: Synthesis, Characterization, Modeling and Optimal Design

Architected materials are multi-phase and cellular materials in which the topological distribution of the phases is carefully controlled and optimized. Nearly two decades of research has resulted in the identification of a number of topologically simple, easy to fabricate, well established topologies, which have been optimized for specific stiffness and strength, impact and blast protection, sound absorption, wave dispersion, active cooling and combinations thereof.

Over the past few years, dramatic advances in processing techniques, including polymer-based templating (e.g., stereolithography, photopolymer waveguide prototyping, two-photon polymerization) and direct single- or multi-material formation (e.g., direct laser sintering, deformed metal lattices, 3D weaving and knitting), have enabled fabrication of new architected materials with arbitrarily complex architectures and remarkably precise control over the geometric arrangement of solid phases and voids from the nanometer to the centimeter scale.

The ordered, topologically complex nature of these materials and the degree of precision with which their features can now be defined suggests the development of new multi-physics multi-scale modeling tools that can enable optimal design. The result is efficient multi-scale cellular materials with unprecedented ranges of density, stiffness, strength, energy absorption, porosity/permeability, chemical reactivity, wave/matter interaction and other multifunctional properties, which promise dramatic advances across important technology areas such as lightweight structures, functional coatings, bio-scaffolds, catalyst supports, photonic/phononic systems and other applications.

Topics addressed in this focus issue will include (but not be limited to):

- ◆ Advances in solid free-form manufacturing (e.g., stereolithography, SLS, SLA, new direct write techniques, etc.)
- ◆ Novel parallel and batch processing techniques for scalable manufacturing
- ◆ 3D weaving, knitting and other fiber forms/preforms
- ◆ Scalable self-assembly techniques
- ◆ Optimization of architectural topology (structure-to-property relations)
- ◆ Inverse methods (function-to-structure)
- ◆ Multi-scale testing (e.g., linking constituent, topological and bulk properties)
- ◆ 3D tomography and related techniques
- ◆ Modeling of non-linear mechanical/physical response
- ◆ Applications of optimal architected materials

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Submission Deadline—August 1, 2017

Electrocatalysts for Oxygen and Hydrogen Evolution

All future synthetic fuels, including solar fuels, will contain hydrogen as an essential element. Electrochemical water splitting is taking center stage as a promising large-scale platform for the production of pure hydrogen, a transportation fuel and commodity for the chemical industry. Electrocatalysts play a central role in electrochemical reactors for that purpose.

This Focus Issue will highlight recent developments in electrocatalysts for hydrogen and oxygen evolution reactions, in both fundamental and applied science, from the molecular scale to the reactor and system design.

Contributed papers are solicited in the following areas:

- ◆ Fundamental studies of hydrogen and oxygen evolution reactions
- ◆ Materials design for electrocatalysis
- ◆ Molecular electrocatalysis
- ◆ Heterogeneous electrocatalysis
- ◆ Novel materials, structures, and architectures
- ◆ Synthesis of electrocatalysts
- ◆ Surface and interface properties
- ◆ Advanced *in situ* and *operando* characterization
- ◆ Diagnosis of electrocatalysis
- ◆ Corrosion and degradation
- ◆ Modeling and simulations of electrocatalysis
- ◆ Device integration and photo-driven systems
- ◆ Photoelectrochemistry

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Submission Deadline—September 1, 2017



Advanced Atomistic Algorithms in Materials Science

Atomistic simulation methodologies play an increasingly important role in identifying and characterizing microstructural processes in materials science. Traditional techniques, such as classical or *ab initio* molecular dynamics, suffer from severe limitations in accessible time scales, length scales, or accuracy, which makes direct comparison with experiments difficult. These limitations call for the development of a richer methodological ecosystem that can enable atomistic simulations over an increasingly large domain of time, size, and accuracy.

Recent methodological improvements, coupled with ever-increasing computing power, have begun to address this challenge. In systems where the dynamics consist of long periods of uneventful vibrational motion punctuated by rare topological transitions, simulation techniques such as accelerated MD and kinetic Monte Carlo methods can be leveraged to significantly extend simulation timescales. Length-scale limitations can be addressed through atomistic-to-continuum bridging approaches, such as the quasi-continuum method, that allow long-range elastic effects to be captured without dramatically increasing the number of degrees of freedom in the system. And high-accuracy atomistic simulations can be enabled through development in density functional theory (DFT) methods, such as orbital-free DFT, time-reversible *ab initio* molecular dynamics, quasi-continuum DFT, and hybrid quantum/classical modeling.

Research papers are solicited in the development or use of innovative methods that push the boundaries of atomistic simulations in materials science. Papers concerning novel atomistic methods that are uniquely able to leverage modern computer architectures are also encouraged.

Contributed articles are sought in the following areas:

- ◆ Techniques for long-time atomistic simulations
- ◆ Techniques for large-size atomistic simulations
- ◆ Techniques that extend the reach of high-accuracy (e.g., DFT) simulations in materials science
- ◆ Scale-bridging atomistic techniques that simultaneously extend simulations capabilities along multiple axes of time, size, or accuracy
- ◆ Applications of advanced atomistic methods to materials science

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