

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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To be considered for this issue, new and previously unpublished results significant to the development of this field should be presented. The manuscripts must be submitted via the *JMR* electronic submission system by **September 1, 2017**. Manuscripts submitted after this deadline will not be considered for the issue due to time constraints on the review process. Please select "Focus issue: *Advanced Atomistic Algorithms in Materials Science*" as the manuscript type. **Note our manuscript submission minimum length of 6000 words, with a maximum of 6-8 figures. Review articles must be pre-approved by proposal to the Editor-in-Chief. The proposal form and author instructions may be found at www.mrs.org/jmr-instructions.** All manuscripts will be reviewed in a normal but expedited fashion. Papers submitted by the deadline and subsequently accepted will be published in the Focus Issue. Other manuscripts that are acceptable but cannot be included in the issue will be scheduled for publication in a subsequent issue of *JMR*.

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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—October 1, 2017

Porous Carbon and Carbonaceous Materials for Energy Conversion and Storage

Carbon and carbonaceous materials including morphologically diverse structures such as zero-dimensional graphene quantum dots, one dimensional nanotubes, two dimensional graphene and three-dimensional polymer monoliths are gaining a great deal of attention due to their unique and tunable electronic and structural properties. These materials can be used on their own (e.g., supercapacitor electrodes) or as supporting scaffolds for other functional materials (e.g., catalysts) for energy conversion and storage. Creation of pores has led to the significant advancement of associated technologies as well as substantial enhancement in performance of the corresponding devices.

This *JMR* Focus Issue will present a broad range of topics covering the synthesis, characterization and applications of porous carbon and carbonaceous materials. Both original research articles and reviews dedicated to the demonstration of the versatile roles of these materials in energy conversion and storage will be considered.

Contributed articles are sought in the following areas:

- ◆ Synthesis and mechanical/electronic/morphological characterizations of porous carbon and carbonaceous materials
- ◆ Theoretical studies illustrating the mechanism of interfacial interactions or reactions between materials and other phases
- ◆ Applications of porous carbon and carbonaceous materials (including their composites) in:
 - ◆ Electrochemical/photonic catalysis
 - ◆ Photoelectrochemical water splitting
 - ◆ Fuel cells
 - ◆ Solar cells
 - ◆ Supercapacitors
 - ◆ Batteries
 - ◆ Other carbon-related fields
- ◆ Short reviews of porous carbon and carbonaceous materials preparation and the progress of their applications in energy conversion and storage

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