Journal of MATERIALS RESEARCH
FOCUS ISSUE • MARCH 2018

Submission Deadline—August 1, 2017

CALL FOR PAPERS

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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MANUSCRIPT SUBMISSION

To be considered for this issue, new and previously unpublished results significant to the development of this field should be presented.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 **August 1, 2017.** Manuscripts submitted after this deadline will not be considered for the issue due to time constraints on the review process. **Submission instructions may be found at www.mrs.org/jmr-instructions.** Please select "Focus Issue: *Electrocatalysts for Oxygen and Hydrogen Evolution"* as the manuscript type. **Note our manuscript submission minimum length of 6000 words, with a maximum of 6-8 figures.** 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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Please contact **jmr@mrs.org** with questions.

Journal of MATERIALS RESEARCH
FOCUS ISSUE • APRIL 2018

Submission Deadline—September 1, 2017

CALL FOR PAPERS

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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The Materials Research Society (MRS®) is a not-for-profit scientific association founded in 1973 to promote interdisciplinary goal-oriented basic research on materials of technological importance. Membership in the Society includes over 16,000 scientists from industrial, government, and university research laboratories in the United States and abroad.

The Society's interdisciplinary approach to the exchange of technical information is qualitatively different from that provided by single-discipline professional societies because it promotes technical exchange across the various fields of science affecting materials development. MRS sponsors two major international annual meetings encompassing many topical symposia, as well as numerous single-topic scientific meetings each year. It recognizes professional and technical excellence, conducts tutorials, and fosters technical exchange in various local geographical regions through Section activities and Student Chapters on university campuses.

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MRS is an Affiliated Society of the American Institute of Physics and participates in the international arena of materials research through associations with professional organizations.

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