Journal of MATERIALS RESEARCH
FOCUS ISSUE • MAY 2018

Submission Deadline—October 1, 2017

CALL FOR PAPERS

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

GUEST EDITORS

Tianyu Liu, University of California, Santa Cruz, USA
Yat Li, University of California, Santa Cruz, USA
Marcus Worsley, Lawrence Livermore National Laboratory, USA
Teng Zhai, Nanjing University of Science and Technology, China

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To be considered for this issue, new and previously unpublished results significant to the development of this field should be presented.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 **October 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: *Porous Carbon and Carbonaceous Materials for Energy Conversion and Storage"* 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*.

jmr@mrs.org
Please contact **jmr@mrs.org** with questions.

jmr 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

GUEST EDITORS

Enrique Martinez Saez, Los Alamos National Laboratory, USA
Danny Perez, Los Alamos National Laboratory, USA
Vikram Gavini, University of Michigan, USA
Steven Kenny, Loughborough University, United Kingdom

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 **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*.

jmr@mrs.org
Please contact **jmr@mrs.org** with questions.

MATERIALS RESEARCH SOCIETY®

Journal of Materials Research Founding Sponsors

Allied-Signal Inc.
Xerox Corporation

About the Materials Research Society

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.

MRS journals maintain a proud tradition of editorial excellence in scientific literature. The *Journal of Materials Research*, the archival journal spanning fundamental developments in materials science, is published twenty-four times a year by MRS and Cambridge University Press. *MRS Bulletin* is a premier source for comprehensive research trends and a timely scan of professional activities. *MRS Communications* is a full-color letters and prospectives journal focused on groundbreaking work across the spectrum of materials research. *MRS Energy & Sustainability–A Review Journal* publishes reviews on key topics in materials research and development as they relate to energy and sustainability. *MRS Advances* is a peer-reviewed online-only journal featuring impactful and emerging research, designed to reflect the way materials researchers work, write, publish and share their results.

The *Journal of Materials Research* is free electronically to all MRS regular and student members. See inside front cover for subscription rates for *Journal of Materials Research.*

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.

For further information on the Society's activities, contact MRS Headquarters, 506 Keystone Drive, Warrendale, PA 15086-7573; telephone (724) 779-3003; fax (724) 779-8313.

Journal of MATERIALS RESEARCH

A publication of the
MRS MATERIALS RESEARCH SOCIETY
Advancing materials. Improving the quality of life.

Periodical Rate Postage Paid at New York, NY
and Additional Mailing Offices

Postmaster—Send change of address notice to:

Cambridge University Press
One Liberty Plaza, 20th Floor,
New York, NY 10006

ISSN: 0884-2914