Special Issue

Multiscale Modeling of Energy Materials

Message from the Guest Editors

The transition from fossil energy sources to renewable and clean energy sources requires a new generation of advanced materials for low-carbon energy technologies. Numerical modeling and computational simulations are inevitable parts of modern materials science. In conjunction with experiments, multiscale modeling techniques (from quantum mechanics to device modeling) are needed to gain insight into phenomena that govern material behavior. In addition to conventional computational modeling, state-of-the-art techniques such as data-driven science and artificial intelligence are likely to advance materials research. With ever-increasing computer power and the rapid development of databases, data-driven science has enabled the rational design and development of novel materials. Additionally, machine-learning-aided computational techniques are becoming invaluable and powerful tools in the study and design of matter. It is our pleasure to invite you to submit a manuscript (full papers, communications, and reviews) for this Special Issue of *Materials*.

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Message from the Editor-in-Chief

Materials (ISSN 1996-1944) was launched in 2008. The journal covers twenty-five comprehensive topics: biomaterials, energy materials, advanced composites, advanced materials characterization, porous materials, manufacturing processes and systems, advanced nanomaterials and nanotechnology, smart materials, thin films and interfaces, catalytic materials, carbon materials, materials chemistry, materials physics, optics and photonics, corrosion, construction and building materials, materials simulation and design, electronic materials, advanced and functional ceramics and glasses, metals and alloys, soft matter, polymeric materials, quantum materials, mechanics of materials, green materials, general. *Materials* provides a unique opportunity to contribute high quality articles and to take advantage of its large readership.

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