



materials



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Multiscale Modeling of Energy Materials

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Message from the Guest Editors

Dear Colleagues,

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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Special Issue



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Message from the Editor-in-Chief

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