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Computational Materials Design for Renewable Energy Applications

Guest Editor:

Dr. Ali Ramazani
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Deadline for manuscript submissions:
closed (31 December 2019)

Message from the Guest Editor

Dear Colleagues,

This Special Issue aims to consider computational materials methods to design nanomaterials for clean and efficient energy conversion and storage. It covers first-principles computations, atomistic simulations, and meso-, macro-, and multi-scale algorithms to understand and design multifunctional nanomaterials, heterostructures, and interfaces. The application must focus on sustainable energy such as photovoltaics, photo- and electrochemistry, CO2 capture and conversion, solar fuels, thermoelectrics, batteries, and ultra-low power electronics. Our Special Issue welcomes all submissions from all studies dealing with computational approaches to energy materials.

Dr. Ali Ramazani
Guest Editor

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Editor-in-Chief

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Message from the Editor-in-Chief

Nanoscience and nanotechnology are exciting fields of research and development, with wide applications to electronic, optical, and magnetic devices, biology, medicine, energy, and defense. At the heart of these fields are the synthesis, characterization, modeling, and applications of new materials with lower nanometer-scale dimensions, which we call "nanomaterials". These materials can exhibit unusual mesoscopic properties and include nanoparticles, coatings and thin films, metal–organic frameworks, membranes, nano-alloys, quantum dots, self-assemblies, 2D materials such as graphene, and nanotubes. Our journal, *Nanomaterials*, has the goal of publishing the highest quality papers on all aspects of nanomaterial science to an interdisciplinary scientific audience. All of our articles are published with rigorous refereeing and open access.

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