Special Issue

Theoretical Calculation and Simulation of Energy Materials

Message from the Guest Editor

This Special Issue aims to collect new advances in theoretical investigations on novel energy materials. We encourage the report of supercomputing applications in design and performance prediction on materials for various applications toward energy storage as well as energy conversion, including sensors, supercapacitors, lithium-ion batteries, and so on. Both bulk materials and low-dimensional materials are of interest in this collection. The content may cover electronic structures, microstructural evolution, defect formation and growth, and their influence on physical properties. Discoveries in both new materials and new development in computational methodology and physical models can make significant contributions.

Guest Editor

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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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