



Theoretical Calculation and Simulation of Energy Materials

Guest Editor:

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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.





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Message from the Editor-in-Chief

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