

Special Issue

Recent Advances in Density Functional Theory and Computational Materials Design

Message from the Guest Editors

Nowadays, materials modeling with computational quantum mechanics has become an indispensable component in physics, chemistry and materials science research. Density function theory (DFT) is arguably the most popular and fruitful method for first-principles materials simulations. As the working horse of computational materials science, DFT often serves as a starting point for other first-principles methods, such as density functional perturbation theory, many-body perturbation theory, dynamical mean field theory, etc. With DFT, researchers are able to study a wide range of materials, from molecules to nanodevices to bulk crystals. A lot of physical and chemical properties can be simulated with varying computational cost, such as magnetism, defect formation, carrier dynamics, optical absorption, chemical reaction, etc. Thanks to the efforts of the computational materials community and DFT software developers, improved density functionals and advanced numerical techniques have been helping to increase the predictive power and widen the applicability of the DFT method.

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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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