Special Issue

Density Functional Theory (DFT) Calculation of Materials Properties

Message from the Guest Editors

Recent years have seen an astonishing development in the field of DFT (density functional theory) calculation of the structure and properties of crystalline materials. There are several reasons underlying the present successful application of DFT to materials science: Faster and faster computers, software improvements (in capability, accuracy and user-friendliness), and theory advancement. Based on these three pillars, computing scientists are now able to describe and understand the properties and performance of real (i.e., already-synthesized) materials and to explore the immense realm of the virtual (i.e., not-yet-synthesized) materials in their quest for the best material ever. Indeed, high-throughput techniques for the search of new crystal structures and the screening of band structure traits have become very popular in the field of computational materials science. For further reading, please follow the link to the Special Issue Website at: http://www.mdpi.com/si/materials/density_functional_theory

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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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