Special Issue

Density Functional Theory and Its Applications in Materials Science: A Critical Comparison between Theoretical Modelling of Crystals and Experiments

Message from the Guest Editors

Density functional theory (DFT) is nowadays playing a crucial role in materials science and related disciplines. It mainly lays in its ability to accurately predict many materials properties and/or materials behavior under different external conditions, bringing closer two important communities, i.e., theoreticians and experimentalists. It has become possible due to constantly ongoing developments in DFT and related theoretical methods as well as modern capabilities of high-performance computing facilities to predict materials properties, demanding a comparison between modelling and experimental results. In this sense 'computational experiment ' is able to replace or supports the real experiments with deeper understanding of observed phenomena at atomistic scale. Thus, the present special issue aims at combining analysis of advanced materials modelling and experimental results for vibrational, optical, mechanical, piezoelectric, magnetic, dielectric and thermoelectric properties, X-ray spectra, defects structures and energetics, thermodynamics and phase diagrams.

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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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