

Special Issue

Advances in Density Functional Theory (DFT) Studies of Solids (Second Volume)

Message from the Guest Editor

The aim of this Special Issue is to collect recent advances in the theoretical study of crystalline materials using first principles calculations. The DFT computations play a significant role in the analysis of a wide range of properties such as structural, electrical, optical, mechanical, vibrational, etc. In turn, a comprehensive understanding of the characteristics of materials is necessary to improve their properties. The use of DFT calculations makes it possible to significantly simplify the interpretation of experimental data, and it is clear that complex research should be carried out using both experimental and theoretical approaches, regardless of the scale of the experiment. Thus, it is no doubt that the density functional theory method is one of the most used in materials science. Keywords

- DFT calculations
- solids
- electronic structure
- electronic density of states
- structural properties
- optical properties
- vibrational properties
- magnetic properties
- bulk materials
- 2D materials

Guest Editor

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About the Journal

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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