Special Issue

Density Functional Theory Application on Chemical Calculation

Message from the Guest Editor

Chemical calculations—methods of quantum chemistry—have become an integral part of most chemical research. Chemical calculations make it possible to study chemical processes in detail at the molecular level, to determine ways to improve the required properties and characteristics of chemicals and chemical processes, thereby increasing the effectiveness of experimental research and contributing to scientific and technological progress in general. Modeling chemical processes using an exact numerical solution of the Schrodinger equation for all elementary particles (electrons and nucleons) in a reasonable time is currently impossible. Therefore, various approximations are used that allow us to achieve reliable results without significant loss of their reliability.

Guest Editor

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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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