Special Issue

Materials Science Advancements Through Density Functional Theory

Message from the Guest Editors

Quantum chemical calculations have become a very useful tool in modern chemistry, and they are currently used by researchers in various fields. A great advantage of using computational quantum chemistry is the possibility of describing reaction mechanisms that are not experimentally feasible to perform, but the data provided guarantees the great reliability of the presented data. Moreover, they are the only source of information about the structure and energy of transition states. Their ability to estimate chemical reaction pathways, including transition state energies and connected equilibria, has led researchers to embrace their use in predicting unknown reactions. Nowadays, calculations develop the unknown reactions, catalyst design, and the exploration of synthetic routes to complex molecules.

This Special Issue covers the quantum chemical calculations in different fields. We invite researchers to publish their theoretical research and combine theoretical and experimental articles as well as properties, biological activities, and molecular docking. The submissions of review articles written by experts in this field will also be appreciated.

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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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