Journal of Nanomaterials

Hindawi

Special Issue on

Computational Modeling of Physical and Chemical Properties of Nanomaterials

CALL FOR PAPERS

Computation modeling is a powerful tool to accurately predict and explore the fundamental properties of nanomaterials. In particular, the practical applications of nanostructured system (e.g., in structural engineering, functionalization of nanomaterials, and computational design) rely on the comprehensive understanding of their physical and chemical properties. The recent development of parallel computer clusters offers powerful computational capabilities to calculate the fundamental properties of complex nanostructures and to simulate physicochemical processes. The framework of the Density Functional Theory provides a computational quantum mechanical method to predict the electronic structure of many-body systems with high accuracy, and it is widely used to study the ground states of various nanomaterials. Recent advances in computational modeling of fundamental properties of nanomaterials not only provided better insight into the mechanisms underlying reaction processes, but also facilitated the practical applications of nanostructured systems.

We invite researchers to contribute original research articles as well as review articles that are devoted to the comprehension of intrinsic properties of nanomaterials, the relationship between the structural engineering and the properties of nanomaterials, modeling and simulation of nanodevices, and the modulation of physical chemistry properties of functional nanomaterials. We are particularly interested in articles describing the knowledge of physicochemical processes of nanosystems, the interaction between nanomaterials and environment for the achievement of practical applications, new insight into novel nanomaterials, modulation of properties of nanomaterials by computational design, and recent improvements on computational modeling methods.

Potential topics include, but are not limited to:

- Computational modeling of various nanostructured materials, such as one-, two-, and three-dimensional nanomaterials
- Physical chemistry properties of two-dimensional nanomaterials and their modulation
- Recent improvements on computational modeling methods
- Chemical functionalization of nanomaterials and nanocomposites for potential applications
- Transport properties of nanomaterials for potential applications of nanodevices
- Accurate prediction of nanosystems and proper description of intermolecular interactions (topological insulator, nanomaterials, and their heterostructures, etc.)
- Computational study of surface and interface sciences (interaction between gas and biomolecules on the surface of nanostructured materials)

Authors can submit their manuscripts via the Manuscript Tracking System at http://mts.hindawi.com/submit/journals/jnm/cmpc/.

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