Tentative Outline

Special Thematic Issue for Current Nanoscience

Numerical Modelling of Nanocomposites
Guest Editor: Wu-Gui Jiang

Aims & Scope:

Composite materials have been widely used in aerospace, defense, transportation and other fields due to their excellent comprehensive properties, especially the designability of their properties. Among them, nanocomposites are the most attractive part, so the research on nanocomposites has been put into an important position in the strategic development of new materials in many countries. In order to predict the performance of nanocomposites, it is expensive and inefficient to use only experimental methods, and numerical simulation technology has become an important and effective approach.

***Keywords*:** Nanocomposite; Finite element; Molecular dynamics; Numerical simulation; Mechanical behaviour

Sub-topics:

The sub-topics to be covered within the issue should be provided: Numerical simulation study on prediction of mechanical properties of

- polymer-based nanocomposites,
- metal-based nanocomposites,
- ceramic-based nanocomposites,
- and other types of nanocomposites

Research approaches include molecular dynamics and finite element methods, but not limited to these methods.

Tentative titles of the articles and list of contributors:

1. A novel multilevel modelling framework to design diamond nanothread bundles
2. Numerical modelling on nanomaterials in superlubricity
3. First-principle calculation of electronic structure and mechanical performance of NbMoTaWRe refractory high entropy alloys
4. Numerical simulation of mechanical characteristics of CNT-reinforced metallic glass nanocomposites
5. Atomistic simulation of ductility enhancement in metal oxide coated silicon nanowires for Li-Ion battery anodes
6. Investigation on crack propagation in nanocomposties using bond-based peridynamics with a new damage model
7. Atomic investigation of rubber-like behaviour in micro-sized pyrolytic carbon

Schedule:

- Manuscript submission deadline: December 2020

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