Special Issue

First-Principle and Atomistic Modelling in Materials Science

Message from the Guest Editor

Theoretical calculations and computer simulations are very important methods to improve our understanding of atomic-level processes in materials and to extend our knowledge on their static, dynamic, kinetic, and thermodynamic properties. Furthermore, the response of the material to external pertubations, in particular mechanical or thermal load and irradiation, can be studied using such computational techniques. This Special Issue of *Materials* shall include articles dealing with applications of first-principle density functional theory (DFT) and atomistic modelling based on interatomic potentials (AM). Both techniques are widely used to investigate ground state properties, finite-temperature effects, and dynamic processes. The present issue shall also include publications in which such a combination of the different computational methods is presented and be focused on solid inorganic materials with a crystalline or amorphous structure. Short communications on recent results, original research articles, as well as reviews may be submitted.

Guest Editor

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Deadline for manuscript submissions

closed (31 December 2020)

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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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