Special Issue

Computational Modelling and Design of Novel Engineering Materials

Message from the Guest Editors

Discovering new materials is an important direction for the development of science worldwide. The use of advanced numerical models makes it possible to reduce the time required for developing and obtaining novel materials with predefined mechanical, thermal, optical, or electronic properties. Computer methods not only allow the determination of material properties at nano, micro, and macro scales, but also allow for multi-scale analyses of phenomena occurring in those materials at various time and length scales. Methods like ab initio including DFT, MD, MC, and CA but also FEM, BEM, or FDM are some of the most commonly used in the analysis of direct problems. Designing new materials often requires the selection of appropriate chemical composition, thermomechanical treatment, or shape of microstructural features, as well as their topology. These tasks can be solved using inverse techniques based on both global and local optimization algorithms. This Special Issue welcomes the submission of all papers in which aspects of the computer modeling of new materials are discussed.

Guest Editors

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Deadline for manuscript submissions

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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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