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Computational Modelling and Design of Novel Engineering Materials

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Deadline for manuscript submissions:
closed (20 April 2022)

Message from the Guest Editors

Dear Colleagues,

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.

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Special Issue

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Message from the Editor-in-Chief

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