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First-Principle and Atomistic Modelling in Materials Science

Guest Editor:

Dr. Matthias Posselt
HZDR - Helmholtz-Zentrum Dresden-Rossendorf, Dresden, Germany

Deadline for manuscript submissions:
closed (31 December 2020)

Message from the Guest Editor

Dear Colleagues,

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.

Dr. Matthias Posselt
Guest Editor

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Message from the Editor-in-Chief

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