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Modelling Materials and Devices at Atomistic Level

Guest Editor:

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Message from the Guest Editor

In the past few years, atomistic simulations have become essential tools for exploring new materials and investigating the working principles of novel electronic devices. The success of ab initio methods based on the density functional theory (DFT) ensures valuable guidance for the synthesis of proper candidates. Complementary, molecular dynamics simulations are able to cover mechanical properties at significantly larger timescales and system sizes. In addition, in recent years, machine learning (ML) techniques combined with atomistic descriptions have boosted the search for new materials and the optimization of device properties.

This Special Issue shall cover topics concerning the modeling of materials and devices at atomistic level. These shall be focused but not limited to materials and interfaces for opto-electronic applications, spin and charge transport in atomic-scale devices, and novel ML approaches coupled to ab initio approaches.

- density functional theory
- electronic structure calculations
- molecular dynamics
- machine learning
- spin and charge transport
- atomic-scale devices
- ab initio modeling of interfaces
- molecular dynamics simulations

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Message from the Editor-in-Chief

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