Special Issue

Challenges and Opportunities in Computational Materials Science

Message from the Guest Editor

The time span between the digital design of materials and their real-world application is decreasing as we better understand complex interactions occurring at the atomic scale and within the bulk of materials. Computational Materials Science (CMS), fueled by high-performance computing, expedites new research that contributes to this progress, thus enabling the scalable design of custom-made materials with decreasing computational costs and increasing efficiency. Knowing that materials are essential to all aspects of modern life, including energy and environmental engineering, chemistry, infrastructure, pharmaceutical design, and more, interdisciplinary collaborations must be encouraged. This Special Issue welcomes the submission of high-quality research focused on the intricacies within the digital design of materials. Topics of interest include, but are not limited to, the following:

- Challenges in the conceptual advancement of existing and the development of new simulation techniques for materials design.
- Novel insights into the behavior and interfacial phenomena of materials.
- Structure–property relationships informed by materials informatics.

Guest Editor

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Message from the Editor-in-Chief

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