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Molecular Dynamics Simulations in Nanomaterials

Guest Editor:

Prof. Dr. Te-Hua Fang
Department of Mechanical Engineering, National Kaohsiung University of Science and Technology, Kaohsiung, 807, Taiwan

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Message from the Guest Editor

Nanomaterials are the leading material and structures in use. This is due to their unique properties, such as high strength, toughness, electrical, thermal conductivity, and mechanical property. The combination of these specific features makes nanomaterials attractive for a broad spectrum of applications in different strategic sectors, namely, aerospace, automotive, mold, tribology, mechanical, and structural industries, among others. Molecular dynamics simulation brings the most significant papers concerned with applications of simulation in nanostructures and nanomaterials, and original contributions to the development of simulation methodology from engineering, materials science, and physics.

The goal of this Special Issue is to cover all aspects of research related to, or of importance to, molecular modeling and simulation of nanomaterials.

In particular, the topics of interest include but are not limited to:

- Graphene and related 2D materials;
- Amorphous and nanocrystalline materials;
- Nanocomposite;
- Porous nanomaterials and its applications
- Mechanical property or thermal conductivity of nanostructures and nanomaterials;
- Phase transformations of nanomaterials.

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Prof. Dr. Wei Pan
State Key Laboratory of New Ceramics and Fine Processing, School of Materials Science & Engineering, Tsinghua University, Beijing 100084, China

Dr. Emerson Coy
NanoBioMedical Centre, Adam Mickiewicz University in Poznań, ul. Wszechnicy Piastowskiej 3, 61-614 Poznań, Poland

Message from the Editorial Board

Now more than ever, research is asked to deliver knowledge and technologies to solve the major challenges faced by our society. The development of new materials and devices for (without the ambition to be exhaustive) energy, health and food technology, together with the need for establishing processes that reduce the impact on critical resources and the environment, is indeed in the spotlight of most contemporary research. Surface science and engineering play a key role in this regard, with an incredible potential in delivering new and deep scientific understanding and technical solutions essential to solve most of the major societal challenges.

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Contact Us

Coatings Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland

Tel: +41 61 683 77 34
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