Special Issue

Molecular Dynamics in Materials Science, Heat Conduction and Nanofluids

Message from the Guest Editors

This Special Issue is devoted to the application of the molecular dynamics (MD) method in materials science, heat conduction, and nanofluids. Molecular dynamics offers a modern and powerful computational method applied to the product design of optimized materials, heat conduction, and flow characteristic of nanofluids. Material systems of industrial interest are highly heterogeneous and are characterized by a variety of defects, interfaces, and other microstructural features (due to the complexity of structural hierarchies on different scales), controlled by phenomena at the nanoscale that can be elucidated by molecular dynamics simulations. MD can be developed or combined with various simulations (such as direct simulation Monte Carlo, kinetic Monte Carlo, meshless methods, etc.) for a range of applications. In this Special Issue, we invite submissions exploring cutting-edge research and recent advances in the fields of materials science, heat conduction, and nanofluids. Both theoretical and experimental studies are welcome, as well as comprehensive reviews and survey papers.

Guest Editors

Dr. Ştefan Ţălu

The Directorate of Research, Development and Innovation Management (DMCDI), The Technical University of Cluj-Napoca, Constantin Daicoviciu Street, No. 15, 400020 Cluj-Napoca, Romania

Dr. Mihai Ţălu

Faculty of Mechanics, University of Craiova, Calea Bucureşti Street, no. 107, 200512 Craiova, Dolj county, Romania

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Applied Sciences
Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland
Tel: +41 61 683 77 34
applsci@mdpi.com

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Message from the Editor-in-Chief

As the world of science becomes ever more specialized, researchers may lose themselves in the deep forest of the ever increasing number of subfields being created. This open access journal *Applied Sciences* has been started to link these subfields, so researchers can cut through the forest and see the surrounding, or quite distant fields and subfields to help develop his/her own research even further with the aid of this multi-dimensional network.

Editor-in-Chief

Prof. Dr. Giulio Nicola Cerullo
Dipartimento di Fisica, Politecnico di Milano, Piazza L. da Vinci 32, 20133 Milano, Italy

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