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Atomistic Simulations under Extreme Conditions

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Deadline for manuscript submissions:
closed (31 December 2022)

Message from the Guest Editor

Dear Colleagues,

Materials under extreme conditions have been revolutionized in the past few years due to technological breakthroughs, e.g., diamond anvil cell and shock wave compression. The response of materials to the broad range of such conditions provides insight into new phenomena, exposes failure modes that limit technological possibility, and presents novel routes for making new materials.

However, it is still challenging to observe the microstructure evolution under extreme conditions from an experimental viewpoint. The atomistic simulation method, i.e., molecular dynamics simulation, is an effective tool to study the effect of specific nanostructural features on the overall mechanical behavior of the material. Thus, the evolution of the microstructure, potential deformation mechanisms, and other related properties under extreme conditions can be studied.

This Special Issue aims to publish papers that advance the field of atomistic simulation methods to discover new materials and investigate existing metal materials under extreme conditions.

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Message from the Editorial Board

Metallic materials play a vital role in the economic life of modern societies; contributions are sought on fresh developments that enhance our understanding of the fundamental aspects related to the relationships between processing, properties and microstructure – disciplines in the metallurgical field ranging from processing, mechanical behavior, phase transitions and microstructural evolution, nanostructures, as well as unique metallic properties – inspire general and scholarly interest among the scientific community.

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Journal Rank: JCR - Q2 (Metallurgy and Metallurgical Engineering) / CiteScore - Q1 (Metals and Alloys)

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