

Special Issue

Atomistic Simulations under Extreme Conditions

Message from the Guest Editor

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.

Guest Editor

Prof. Dr. Wangyu Hu

College of Materials Science and Engineering, Hunan University,
Changsha 410082, China

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

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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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Prof. Dr. Hugo F. Lopez

Department of Materials Science and Engineering, College of Engineering & Applied Science, University of Wisconsin-Milwaukee, 3200 N. Cramer Street, Milwaukee, WI 53211, USA

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Beijing Advanced Innovation Center of Materials Genome Engineering, State Key Laboratory for Advanced Metals and Materials, University of Science and Technology Beijing, 30 Xueyuan Road, Beijing 100083, China

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