Special Issue

Progress in Nuclear Material Simulation Research

Message from the Guest Editor

This Special Issue, titled “Progress in Nuclear Material Simulation Research”, aims to explore cutting-edge advancements in computational simulations of nuclear materials. Nuclear materials face harsh service environments, posing significant challenges for experimental research, particularly due to safety and regulatory issues related to radioactive substances, as well as limitations in high-purity sample preparation and characterization, exemplified by the difficulties encountered in experimental studies of uranium metal. This Special Issue focuses on computational modeling of irradiation behavior in nuclear fuels, offering insights into structural integrity and performance degradation under extreme conditions. Furthermore, it delves into computational studies on the separation and enrichment of radionuclides, with a focus on utilizing first-principles and molecular dynamics simulations to investigate MXene materials for adsorbing and separating radionuclide ions, thereby providing innovative strategies for nuclear waste management and material recycling.

Guest Editor

Dr. Yujuan Zhang

School of Materials Science and Engineering, University of Science and Technology Beijing, Beijing 100083, China

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

mdpi.com/journal/materials

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Materials (ISSN 1996-1944) was launched in 2008. The journal covers twenty-five comprehensive topics: biomaterials, energy materials, advanced composites, advanced materials characterization, porous materials, manufacturing processes and systems, advanced nanomaterials and nanotechnology, smart materials, thin films and interfaces, catalytic materials, carbon materials, materials chemistry, materials physics, optics and photonics, corrosion, construction and building materials, materials simulation and design, electronic materials, advanced and functional ceramics and glasses, metals and alloys, soft matter, polymeric materials, quantum materials, mechanics of materials, green materials, general. *Materials* provides a unique opportunity to contribute high quality articles and to take advantage of its large readership.

Editor-in-Chief

Prof. Dr. Maryam Tabrizian

1. Department of Biomedical Engineering, Faculty of Medicine and Health Sciences, McGill University, Montreal, QC H3A 2B6, Canada
2. Faculty of Dentistry and Oral Health Sciences, McGill University, 3640 Rue University, Montreal, QC H3A 0C7, Canada

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