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First-Principles Studies and Electronic Structures of Nano-Scale Materials

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Deadline for manuscript submissions:
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Message from the Guest Editor

This Special Issue explores the fascinating field of nano-scale materials, focusing on their crystalline structures, alloys, and applications in nuclear materials and nuclear energy. For this, we are seeking the submission of original research, reviews, and perspectives utilizing density functional theory (DFT), ab initio molecular dynamics (AIMD), and other first-principles-based theoretical frameworks to investigate electronic structures and properties.

Nano-scale materials possess unique properties due to their reduced dimensions, making them appealing for nuclear applications. First-principles calculations provide insights into atomic-scale behavior, and this Special Issue aims to enhance our understanding of the relationship between crystalline structures, alloys, and the performance of nano-scale materials in nuclear systems.

We invite researchers, and experts to contribute their original research on nano-scale materials for nuclear materials and nuclear energy applications. The aim of this Special Issue is to foster interdisciplinary collaborations and advance our understanding of nano-scale materials in the context of nuclear science and technology.

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Message from the Editor-in-Chief

Welcome to *Crystals*, the journal dedicated to the fascinating world of crystallographic research! Crystals are more than mere decorative elements; they hold the key to understanding the fundamental structure of matter. Our mission is to explore the crucial significance of this research across various fields. From medicine to technology, chemistry to geology, crystals play a vital role. Their structure provides insights into new advanced materials, innovative drugs, and groundbreaking technologies. Through *Crystals*, we delve into the microscopic world to discover solutions that will shape the future. Join us on a journey through the *Crystals*, where science merges with beauty and innovation.

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