Special Issue

Synthesis, Characterization and Computational Modeling of Nanostructured Materials

Message from the Guest Editors

The realm of nanostructured materials constitutes a cross-disciplinary frontier in material science, bridging quantum mechanics, quantum chemistry, biology, and beyond. These materials exhibit functional, structural, or dual attributes, adopting forms such as layered materials, 2D heterostructures, micro- and nanoparticles, composites, and others. Their most prominent applications include nanoelectronics, optoelectronics, flexible and quantum electronics, nanomedicine, high-efficiency photocatalysts, and functional textiles. Understanding and developing nanostructured materials necessitates a comprehensive approach, integrating predictive computational modeling, atomic- to nano-scale design, fabrication, and multi-scale characterization. Their swift, effective, and agile design can be enabled through the strategic fusion of high-performance computing (HPC) and machine learning. This Special Issue will highlight the exploration and outcomes of nanostructured material synthesis, delving into their multi-scale characterization and computational modeling in order to establish atomic structure–property relationships and obtain high-performance nanostructures.

Guest Editors

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