Special Issue

Development and Research on Theoretical Chemistry in Materials

Message from the Guest Editor

- This Special Issue is intended to act as a contributor to this discussion and to future developments on this theme. We are pleased to invite you to present cutting-edge research at the intersection of theoretical chemistry and materials science in all classes of materials, highlighting how theoretical and computational approaches are revolutionizing our understanding of material properties, design, and applications. This Special Issue will cover a wide range of topics, including quantum chemical calculations (density functional theory and ab initio methods), molecular dynamics simulations, and machine learning techniques applied to materials research.
- Full papers, communications, and reviews are all welcome. Research areas may include (but are not limited to) the following: novel theoretical methods, predictive modeling of material properties, and computational studies that guide experimental work in materials development.

Guest Editor

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Message from the Editorial Board

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.

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