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Density Functional Theory and Its Applications in Materials Science: A Critical Comparison between Theoretical Modelling of Crystals and Experiments

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Deadline for manuscript submissions:
closed (10 July 2024)

Message from the Guest Editors

Dear Colleagues,

Density functional theory (DFT) is nowadays playing a crucial role in materials science and related disciplines. It mainly lays in its ability to accurately predict many materials properties and/or materials behavior under different external conditions, bringing closer two important communities, i.e., theoreticians and experimentalists. It has become possible due to constantly ongoing developments in DFT and related theoretical methods as well as modern capabilities of high-performance computing facilities to predict materials properties, demanding a comparison between modelling and experimental results. In this sense 'computational experiment ' is able to replace or supports the real experiments with deeper understanding of observed phenomena at atomistic scale. Thus, the present special issue aims at combining analysis of advanced materials modelling and experimental results for vibrational, optical, mechanical, piezoelectric, magnetic, dielectric and thermoelectric properties, X-ray spectra, defects structures and energetics, thermodynamics and phase diagrams.

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Message from the Editor-in-Chief

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