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Density Functional Theory (DFT) Calculation of Materials Properties

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Message from the Guest Editors

Recent years have seen an astonishing development in the field of DFT (density functional theory) calculation of the structure and properties of crystalline materials. There are several reasons underlying the present successful application of DFT to materials science: Faster and faster computers, software improvements (in capability, accuracy and user-friendliness), and theory advancement. Based on these three pillars, computing scientists are now able to describe and understand the properties and performance of real (i.e., already-synthesized) materials and to explore the immense realm of the virtual (i.e., not-yet-synthesized) materials in their quest for the best material ever. Indeed, high-throughput techniques for the search of new crystal structures and the screening of band structure traits have become very popular in the field of computational materials science.

For further reading, please follow the link to the Special Issue Website at:

http://www.mdpi.com/si/materials/density_functional_theory

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Message from the Editor-in-Chief

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