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Density Functional Theory (DFT) of Two-Dimensional Materials

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Deadline for manuscript submissions:
closed (31 October 2023)

Message from the Guest Editors

Density functional theory (DFT) has become one of the most important tools for the theoretical study of materials, including for the most part their electronic structure, as well as their structural, mechanical, magnetic, and other properties. Moreover, it has become a strong tool for the theoretical prediction of materials.

This Special Issue of Crystals "Density Functional Theory (DFT) of Two-Dimensional Materials", aims to become a collection of original research articles utilizing DFT calculations for the study of 2D materials and their properties. We kindly invite contributions to this Special Issue on a wide range of topics, including, but not limited to, the following:

Theoretical discovery of novel 2D materials with exotic properties;
Structural, mechanical, electronic, magnetic, optical, and transport properties of 2D materials;
Nanoflakes and nanoribbons of 2D materials;
Edge properties of 2D materials;
The effect of structural distortions or doping on 2D materials' properties;
Surface reactivity;
Applications of 2D materials for energy or environmental applications;
One-dimensional and three-dimensional materials based on 2D structures.

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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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