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Applications of Density Functional Theory in Crystalline Materials

Guest Editor:

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Deadline for manuscript submissions:
closed (13 November 2023)

Message from the Guest Editor

Dear Colleagues,

Rapid advances are taking place in the application of density functional theory (DFT) to describe the structures and properties of crystalline materials. DFT remains one of the most effective computational tools owing to its strong predictive powers for the crystal structures, physical and chemical properties, and its ability to accurately treat complex surfaces and interfaces.

The special issue will publish original and review articles or communications of preliminary but significant or inspiring results which demonstrate current research topics or directions. This issue aims at gathering articles that highlight some of the following topics:

(1) The novel theory, approach and its application resolving the physical and chemical issues of crystals of importance within the framework of DFT;

(2) Application of DFT on resolving structure-property relationship in crystalline materials;

(3) Design of new crystal structures and new functional features by the use of DFT.

https://www.mdpi.com/journal/molecules/special_issues/Density

We believe that you could make an excellent contribution to this Special Issue.

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Editor-in-Chief

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Message from the Editor-in-Chief

As the premier open access journal dedicated to experimental organic chemistry, and now in its 25th year of publication, the papers published in *Molecules* span from classical synthetic methodology to natural product isolation and characterization, as well as physicochemical studies and the applications of these molecules as pharmaceuticals, catalysts and novel materials. Pushing the boundaries of the discipline, we invite papers on multidisciplinary topics bridging biochemistry, biophysics and materials science, as well as timely reviews and topical issues on cutting edge fields in all these areas.

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