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Density Functional Theory Application on Chemical Calculation

Guest Editor:

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Deadline for manuscript submissions:
closed (20 December 2023)

Message from the Guest Editor

Chemical calculations—methods of quantum chemistry—have become an integral part of most chemical research. Chemical calculations make it possible to study chemical processes in detail at the molecular level, to determine ways to improve the required properties and characteristics of chemicals and chemical processes, thereby increasing the effectiveness of experimental research and contributing to scientific and technological progress in general. Modeling chemical processes using an exact numerical solution of the Schrodinger equation for all elementary particles (electrons and nucleons) in a reasonable time is currently impossible. Therefore, various approximations are used that allow us to achieve reliable results without significant loss of their reliability.

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Message from the Editor-in-Chief

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