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## Recent Advances in Density Functional Theory and Computational Materials Design

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Deadline for manuscript submissions:

**closed (20 November 2023)**

### **Message from the Guest Editors**

Nowadays, materials modeling with computational quantum mechanics has become an indispensable component in physics, chemistry and materials science research. Density function theory (DFT) is arguably the most popular and fruitful method for first-principles materials simulations. As the working horse of computational materials science, DFT often serves as a starting point for other first-principles methods, such as density functional perturbation theory, many-body perturbation theory, dynamical mean field theory, etc. With DFT, researchers are able to study a wide range of materials, from molecules to nanodevices to bulk crystals. A lot of physical and chemical properties can be simulated with varying computational cost, such as magnetism, defect formation, carrier dynamics, optical absorption, chemical reaction, etc. Thanks to the efforts of the computational materials community and DFT software developers, improved density functionals and advanced numerical techniques have been helping to increase the predictive power and widen the applicability of the DFT method.



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## Message from the Editor-in-Chief

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