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# Recent Advances in Density Functional Theory and Computational Materials Design

Guest Editors:

**Dr. Meng Wu**
Department of Physics, University of California at Berkeley, 366 Physics North MC 7300, Berkeley, CA 94720-7300, USA

**Dr. Yalun Yu**
Schrödinger, Inc., University of Maryland, College Park, MD, USA

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## 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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**Prof. Dr. Maryam Tabrizian**
1. Department of Biomedical Engineering, Faculty of Medicine and Health Sciences, McGill University, Montreal, QC H3A 2B6, Canada
2. Faculty of Dentistry and Oral Health Sciences, McGill University, 3640 Rue University, Montreal, QC H3A 0C7, Canada

## Message from the Editor-in-Chief

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## Contact Us

*Materials* Editorial Office
MDPI, Grosspeteranlage 5
4052 Basel, Switzerland

Tel: +41 61 683 77 34
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