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Special Issue on

Density Functional Theory Computations of Advanced Materials

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The past few years have seen the rapid development of density functional theory computation, as well as its utilization in investigating the chemical properties of advanced materials for various applications. These applications include clean-energy conversion/storage (such as fuel cell, water-splitting, solar cell, and battery), nanodevices, optoelectronics, photocatalysis, and electrocatalysis.

This special issue aims at creating a forum of discussion on recent progresses of advanced materials in the above mentioned applications by density functional theory simulations.

Potential topics include but are not limited to the following:

- Metal and metal-alloys
- Porous materials
- 2D nanomaterials
- Nanowire and Nanotube
- Quantum dot
- Related methodological advancement

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