

Special Issue

Computational Catalysts and Materials Design for Energy Conversion and Storage

Message from the Guest Editor

Here, in this Special Issue, we identify three frontiers and challenging areas in computational catalyst and materials design for energy conversion and storage:

development of new computational methods/approaches for energy catalysis;
computational studies of the heterogeneity of the catalytically active sites;
data science-enabled computational modeling of catalysts/materials properties and catalytic reaction pathways.

This Special Issue intends to highlight the recent advances of computational methods and approaches for studying challenging problems of catalysts and materials in energy conversion and storage. Both research and review articles are welcome.

Guest Editor

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closed (20 March 2022)



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Editor-in-Chief

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