Special Issue

Advanced Functional Materials Design and Computation

Message from the Guest Editors

The Special Issue on **Advanced Functional Materials Design and Computation** showcases cutting-edge developments in density functional theory (DFT), machine learning (ML), and machine-learned atomic potentials for the design of functional materials and catalysts aimed at advancing sustainable chemistry. This issue addresses critical global challenges in energy and environmental sustainability by highlighting how computational and machine-learning techniques are accelerating the development of innovative materials and catalytic systems. Topics for this Special Issue include materials for solar cells and thermoelectrics aimed at improving energy harvesting and conversion efficiency. This issue also encompasses advanced catalytic systems for hydrogen production and ammonia synthesis, with a focus on green and energy-efficient processes. Further, it explores recent progress in CO2 capture and conversion technologies, alongside catalytic strategies for biomass valorization to produce renewable fuels and chemicals.

Guest Editors

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Editor-in-Chief

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