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Computational and Theoretical Methods in Environmental Catalysis

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Message from the Guest Editors

This Special Issue of "Computational and Theoretical Methods in Environmental Catalysis" focuses on advancing our understanding and application of computational and theoretical approaches in catalysis for environmental remediation. Specifically, it explores the utilization of advanced computational techniques to design and optimize catalysts for environmental applications, with a particular emphasis on catalytic processes aimed at mitigating environmental pollution and promoting sustainability.

Through a collection of original research articles, reviews, and perspectives, this Special Issue provides an opportunity for researchers to exchange ideas, share insights, and showcase the latest developments in the field. Topics covered include the computational modeling of catalytic mechanisms, structure–property relationships in catalytic materials, simulation of reaction kinetics and dynamics, and development of predictive models for catalyst design and optimization.

Deadline for manuscript submissions:
30 November 2024

mdpi.com/si/205791

Special Issue