

Special Issue

Advances in Sustainable Remediation Technologies: Advanced Oxidation, Catalytic Nanomaterials, and Computational Modeling

Message from the Guest Editors

The presence of pharmaceuticals in the environment poses a significant challenge due to their potential ability to harm ecosystems and human health. Conventional removal methods are often unable to completely eliminate these pharmacologically active compounds. However, sustainable catalysis has emerged as a promising solution, offering the effective degradation and mineralization of these compounds via advanced oxidation processes. Heterogeneous catalysis, in particular, has garnered attention for its ability to utilize novel materials with unique catalytic properties. Despite its potential, the widespread application of these materials is hindered by high costs. Computational modeling, including ab initio calculations and molecular dynamics simulations, emerges as a crucial tool in optimizing the performance of catalysis and predicting the behavior of compounds, thus mitigating the economic barriers to its large-scale implementation.

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