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Computational Catalysis for Sustainability

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Message from the Guest Editors

Dear Colleagues,

The past decade has seen exponential progress in computational speed and the development of robust software tools. Incorporating cutting-edge machine learning and descriptor-based methods has further propelled the exploration of catalyst screening, enabling the identification of promising candidates for sustainable catalysis with unparalleled efficiency. As computational catalysis continues to evolve, its impact on clean energy solutions and sustainability is expected to become ever more profound.

This Special Issue aims to publish original computational-based investigations and reviews within the broad field of catalysis. This includes the development of new computational techniques and screening methods, as well as the rigorous application of current computational tools for discovering new catalysts, reaction mechanisms, or catalytic processes. All fields of catalysis that are driven by a substantial computational component, including, but not limited to, heterogeneous, homogeneous, organocatalysis, biocatalysis, photocatalysis, electrocatalysis, and environmental catalysis, will be considered.