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Metal Catalyst Discovery, Design and Synthesis

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Message from the Guest Editors

Dear Colleagues,

Catalysts remain an indispensable piece of kit in the synthetic chemist's toolbox that facilitates chemical transformations with efficiency and selectivity. Transition metals and their complexes are considered the pillars of this arena owing to their redox properties and proclivity to facilitate bond breaking and formation steps. Whilst the development of new catalysts with tailored properties often depends on trial-and-error experimentation, these processes are now routinely directed by computational approaches. Advanced nano-synthetic techniques with characterization cutting-edge tools svnergistically coordinate with the established models to lead the designed catalysts to the real world.

This Special Issue delves into the multifaceted realm of catalyst design, exploring state-of-the-art experimental and computational strategies used for the de novo design of catalysts or their optimisation towards enhanced activity, stability, and selectivity. Contributions are invited within a broad thematic scope, including mechanistic studies, process development and synthetic strategies for catalyst design and optimisation.











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Editor-in-Chief

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Message from the Editor-in-Chief

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