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The Powerful Synergy of Computational and Experimental Approaches in Catalysis

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Message from the Guest Editor

Combining both experimental and computational methods is an interdisciplinary approach of great benefits to explain the main features of complex molecular systems involved in chemical areas at the frontiers of chemical sciences, including homogeneous and heterogeneous transition metal catalysis and organo-, photo- and photoredox catalysis. The advances reached within the applied theoretical framework in recent decades, in particular in the case of density functional theory and solvation models, have substantially permitted the explanation of complex mechanistic outcomes of an incremental number of chemical reactions as well as their selectivity.

The present Special Issue intends to publish original research and review articles on the state-of-the-art of experimental and computational synergy in accounting for and exploring reactivity, selectivity and mechanisms in transition metal, organo-, organic photo-, and photoredox catalysis in homo- and heterogeneous phases.