Special Issue

Computational Chemistry and Catalysis: Prediction and Design

Message from the Guest Editors

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 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, stability and mechanisms in transition metal, organo-, organic photo-, and photoredox catalysis in homo- and heterogeneous phases. Submission of articles combining experimental and theoretical approaches are particularly encouraged. Purely computational studies providing new methodologies to be used in synergy with experimental techniques and improving the current mechanistic understanding of catalytic processes will be also considered.

Guest Editors

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Deadline for manuscript submissions

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