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Organocatalysis: Mechanistic Investigations, Design, and Applications

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Message from the Guest Editor

Catalysis remains one of the most challenging topics in contemporary organic chemistry. Because of the absence of transition metals, organocatalytic methods are attractive for the preparation of pharmaceutical compounds where levels of certain metal-ion contamination are tightly controlled. While the asymmetric organocatalysis field is currently growing exponentially, an understanding of the mechanistic details involved in most of these reactions has often lagged far behind the pace of catalyst development, which retards catalyst design. However, over the last two decades, computational methods have become a cost-effective treatment of large chemical systems with reasonable accuracy. Remarkably, density functional theory (DFT) has been especially useful in the field of organic chemistry in order to elucidate the mechanisms behind chemical reactions.

This Special Issue focuses on synthetic and computational organic chemistry and their contributions to enlarge and enhance our understanding of organocatalysis. This will include studying, predicting, understanding, and validating chemical reactivity in catalytic systems.