Special Issue

Advanced Strategies for Catalyst Design

Message from the Guest Editor

Efficient catalysts are expected to be stable, active, and selective. In the past, the development of new catalysts has mainly depended on trial and error, a laborious and time-consuming approach. Nowadays, the mechanistic details of numerous important chemical reactions have been unraveled, and this information is essential to intelligently design novel catalysts. Thus, all the efforts devoted to a deep understanding of an intricate catalytic mechanism and to the preparation of novel catalysts relying on it are priceless. Chemists must set up adequate strategies, merging experimental and computational knowledge and abilities, to tune the performance of molecules that might be successful in the lab. For this Special Issue, researchers are invited to submit original research papers and review articles related to advanced strategies for catalyst design. Topics of interest include but are not limited to the following: The computer-aided design of catalysts;
Weak interactions in catalysis;
Bioinspired catalysis
Big data and catalysis;
Integrated experimental and theoretical approaches to catalyst design.

Guest Editor

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