Special Issue

Computational Methods and Their Application in Catalysis

Message from the Guest Editor

Computational catalysis is a rapidly developing field because of the impressive advancements in the quantum-mechanical techniques and in the speed and power of computers, which enable the elucidation and rationalization of how chemical processes are accelerated by the presence of a catalyst, with unprecedented accuracy. This Special Issue focuses on recent advances in the application of state-of-the-art computational approaches to better understand enzymes and homogeneous or heterogeneous catalysts, and on challenges that still need to be resolved for the ultimate goal of designing novel and/or more efficient catalysts entirely by a computer. Full papers, communications, perspectives, and mini-reviews are most welcome.

Guest Editor

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