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Computational Methods and Their Application in Catalysis

Guest Editor:

Dr. José R. B. Gomes
CICECO—Aveiro Institute of Materials, Department of Chemistry, University of Aveiro, Campus Universitário de Santiago, 3810-193 Aveiro, Portugal

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Message from the Guest Editor

Dear Colleagues,

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.

Dr. José R. B. Gomes
Guest Editor