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

Author Benefits

**Open Access:** free for readers, with publishing fees paid by authors or their institutions.

**High visibility:** indexed by the Science Citation Index Expanded (Web of Science), Scopus and other databases.

**Rapid publication:** Manuscripts are peer-reviewed and a first decision provided to authors approximately 19 days after submission; acceptance to publication is undertaken in 7 days (median values for papers published in this journal in 2016).