Theoretical Modeling of Catalytic Processes: Challenges, Applications and Perspectives

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Message from the Guest Editors

Dear colleagues,

Catalysis remains an actively developing field of science with numerous applications in industry, medicine and everyday life. Assistance from the theory side is often needed to gain a detailed understanding of underlying processes of catalytic processes, optimize them, and suggest possible development directors.

This Special Issue is devoted to capabilities and perspectives of theoretical approaches in catalysis ranging from atom-resolved quantum chemistry to macroscopic models. Our aim is to highlight recent developments and new advancements in this rapidly growing field. Contributions from all fields of catalysis are welcome, including homogeneous, heterogeneous, photo- and electrocatalysis, as well as biocatalytic systems. The potential topics include but are not limited to:

- Modeling of photocatalytic transition metal complexes;

- Theoretical approaches to surfaces and interfaces in catalysis;

- Nanoparticles as catalysts;

- Mass and heat transfer problems in catalysis;

- Coarse-grained and hybrid modeling of catalytic processes.

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