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PREFACE

Preface to the special issue on experiments and theory

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Abstract
In this special issue different strategies in theory and experiments are exposed to understand and explain the physicalchemistry behind Catalysis and Surface Science.

During the last couple of years, due to the pandemic situation, labs around the world were closed for several months and research felt the impact of the lockdown. This scenario was translated to many traditional meetings of catalysis and surface chemistry, which were canceled, postponed or held online.

In this context, much more cooperative studies are needed to have a deeper understanding of catalytic processes and the structure-reactivity relationships that govern the behavior of those systems. During the last decades, instrumental and methodological advances have allowed insights into surface reactions in unprecedented detail. Simultaneously, computational chemistry, particularly in the frame of density functional theory (DFT), has become broadly available with the help of the increasing computing power. The development of DFT-based codes has led to amazing advances in quantum chemistry, especially in its application to surfaces. Nowadays, it is possible to mimic complex systems such as those in catalysis on a routine basis.

However, connecting the results obtained by both theory and experiments, and finding a common language, remain a challenge. Thus, the aim of this special issue is to promote the visibility of research performed as a joint venture between experimentalists and theoreticians in catalysis and surface chemistry.

This issue contains 18 invited research papers on topics of current technological importance. Subjects run from catalytic combustion, electrochemistry, surface processes, advanced characterization techniques and enzymatic reactions. The fundamental chemical-physics aspects of the surface chemistry involved during catalytic processes are assessed, combining traditional catalytic activity measurements, characterization techniques, in situ spectroscopy and molecular modeling.

We would like to kindly thank the authors who contributed to this special issue. All the contributions show the current advances and trends in theory and experiments for catalysis and surface reactions. We also want to thank the editor-in-chief, professor Hans-Joachim Freund, and to the editorial staff of Topics in Catalysis for their help and assistance.

Finally, as guest editors, we expect that this issue contributes to increasing the collaborations between experimental and theoretical research groups.

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