Special Issue

Metal–Oxygen Interfaces in Catalysis and Surface Chemistry: Interactions, Reactivity, and Modeling

Message from the Guest Editors

Metal–oxygen interfaces lie at the heart of many catalytic transformations, providing unique reactivity through complex electronic, geometric, and chemical interactions. These interfaces govern key processes such as oxygen activation, redox cycling, and selective bond breaking or formation, yet their diverse and complex nature hinders our molecular-level understanding of them. This Special Issue will compile cutting-edge experimental and theoretical advances that probe the structure, dynamics, and reactivity of metal–oxide systems at the atomic level. We welcome contributions that explore the fundamental principles of these interfaces and emerging practical opportunities, with the goal of promoting novel strategies related to catalyst design and mechanistic understanding.

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As the premier open access journal dedicated to experimental organic chemistry, and now in its 25th year of publication, the papers published in *Molecules* span from classical synthetic methodology to natural product isolation and characterization, as well as physicochemical studies and the applications of these molecules as pharmaceuticals, catalysts and novel materials. Pushing the boundaries of the discipline, we invite papers on multidisciplinary topics bridging biochemistry, biophysics and materials science, as well as timely reviews and topical issues on cutting edge fields in all these areas.

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