Special Issue

Photoelectrochemical and Photocatalytic Performance: Catalysts for Renewable Energy Production and Wastewater Remediation

Message from the Guest Editors

The Special Issue will focus on the recent advances in photoelectrochemical and photocatalytic performance for direct solar water splitting for hydrogen production, CO2 reduction to chemicals and fuels, degradation of organic substances, and water purification. Results from both theoretical and experimental studies on heterogeneous catalysts are included. The experimental scope includes the synthesis, modification, and applications of group IV, III–V, metal oxides, and earth abundant material-based catalysts which excel in terms of their high photocatalytic activity and that possess tunable physicochemical properties that can be controlled by changing the material composition. The computational scope is on studies of the aforementioned catalysts for various electronic structure calculations, including excited states, polaron and charge transfer studies, band edge alignments at interfaces, and computational reaction network studies that consider the coupling of intermediates within kinetic and Monte Carlo models in addition to their validation through experimental results that allow gaining insights into photo(electro)catalytic behavior at longer time and length scales.

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Deadline for manuscript submissions

closed (10 December 2021)

Catalysts

an Open Access Journal by MDPI

Impact Factor 4.0
CiteScore 7.6

mdpi.com/si/65474

Catalysts
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Editor-in-Chief

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