Special Issue

Computational and Experimental Advances in Photocatalysis

Message from the Guest Editor

This Special Issue will focus on the powerful synergy between computational modeling and experimental research, which is accelerating the development of novel photocatalysts and deepening our understanding of reaction mechanisms. The goal is to highlight the advances driving photocatalysis as a key solution for global energy and environmental challenges. Topics of interest include, but are not limited to:

- Design and Synthesis: Development of novel photocatalysts (heterostructures, quantum dots, MOFs) with enhanced efficiency.
- Mechanisms and Dynamics: Fundamental studies of charge dynamics and photocatalytic reaction mechanisms.
- Computational Modeling: Use of simulations to predict properties and guide material development.
- Advanced Characterization: Application of in-situ and operando techniques to investigate catalysts in action.
- Applications: Innovations in hydrogen (H_2) production, CO_2 reduction, N_2 fixation, and environmental remediation.

We look forward to your valuable contribution to advancing the frontiers of photocatalysis.

Guest Editor

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