



Novel Photocatalytic Materials: Computational Simulation and Design of the Structure, Properties, and Catalytic Mechanism

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Message from the Guest Editor

Photocatalysts have been widely applied today in various areas such as water splitting, wastewater treatment, air purification, and bacteria inactivation. It is a challenge of great importance to explore newer photocatalysts that are stable, abundant, and efficient. In recent years, intensive efforts have been devoted to the discovery of novel photocatalytic materials (e.g., C/N/S-doped TiO₂, complex metal oxides, and low-dimensional semiconductor photocatalysis), to understand the fundamental principles governing the photocatalytic performance, improve efficiency, and expand the scope of applications.

In this collection, we are particularly interested in designing and identifying structures and properties with advanced photocatalytic performance. Additionally, we aim to rationalize the intrinsic properties and features affecting photocatalytic performance and further insight into their catalytic mechanism via simulation and calculation.

