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Photocatalytic Modeling for Maximizing Utilization of Real-Time Changing Sunlight and Rationalizing Evaluation

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Abstract

Because of very high potential barrier for thermionic emission and trap-assisted charge recombination, photocatalytic reaction rate that determined by semiconductor-cocatalyst interfacial electron transfer severely deviates from linearity to the photocatalyst dosage or to the light intensity. This makes it challenging to maximize utilization of practical irradiation by referring the parameters evaluated from method used in conventional catalysis. We here develop a model and predict that photocatalytic reaction rate positively correlates to photocatalyst concentration under weak illumination while the correlation becomes negative under intense irradiation. The theoretical simulation that matches the experimental values can be used to guide maximizing photocatalytic photon utilization under various intensity of irradiation. The strong correlation can rationalize photocatalytic evaluation instead of obtaining a numerically high value by excessively lowering the denominators. To realize efficient utilization of real-time changing sunlight, we propose a reactor configuration that can optimize the amount of photocatalyst participating into the reaction.

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