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Editorial

Editorial: Semiconductor Photocatalysts

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Since the discovery of the photocatalytic ability of TiO_2 electrodes to decompose water [1], techniques of semiconductor photocatalysis, including photocatalytic energy conversion and photocatalytic pollution treatment, have achieved rapid development. In the contemporary world, these concerns animate the interdisciplinary fields of semiconductor physics, materials science, environmental and energy science, computational chemistry and many others [2–9]. The overall photocatalysis process typically incorporates light absorption, charge generation/separation/transfer, and surface redox reactions [5,6]. These three steps are complementary and indispensable, and only when they executed with a high degree of efficiency can the overall photocatalytic efficiency be high. A series of strategies, such as foreign element doping [10,11], metal loading [12], heterojunction construction [13,14], strain and external electric field regulation [15,16], have been developed to overcome the bottlenecks of each step in order to improve the photocatalytic efficiency. In this Special Issue of *Crystals*, entitled "Semiconductor Photocatalysts", we have collected a total of 4 articles about the recent progress in semiconductor photocatalysis. Next, we briefly outline the research highlights of these studies.

Alhalili et al. [17] studied the effect of calcination time on TiO_2 nanoparticles (NPs), prepared from Aloe vera leaf extract, when the temperature was maintained at 500 °C and discussed the relationship between calcination time and the size of NP. The size of synthesized TiO_2 NP decreases with the increase in calcination time. The NP with small size possesses improved optical and photocatalytic activity. The visible light photocatalytic ability for RR180 degradation varies with time, from 1 h with TiO_2 NP (23 ± 2 nm) to 2 h with TiO_2 NP (83 ± 5 nm).

Xiao et al. [18] used molten salt and ultrasound-assisted liquid-phase exfoliation methods to successfully prepare a black phosphorus-/heptazine-based crystalline carbon nitride (BP/KPHI) composite. The photocatalytic hydrogen production performance of BP/KPHI composites can be tuned by altering the mass ration of BP. The 10% BP/KPHI composite shows the highest photocatalytic hydrogen production rate of 4.3 $mmol \cdot g^{-1} \cdot h^{-1}$, which is about three times higher than that of KPHI. The excellent photocatalytic performance of BP/KPHI composite can primarily be attributed to the stellar photoinduced carrier separation and excellent visible light harvesting capacity.

First-principles calculation based on density functional theory (DFT) plays an undeniable role in developing and designing novel semiconductor photocatalysts. Li et al. [19] adopted first-principles calculation methods to investigate the geometric, electronic, optical properties as well as the hydrogen evolution reaction (HER) and carrier mobility of SiP_2 monolayers (MLs) in order to explore their potential use in photocatalytic hydrogen production. SiP_2 MLs are indirect bandgap semiconductors with 2.277 bandgaps that are still stable at 1200 K. The suitable band edge alignment and strong light absorption ability make SiP_2 MLs into potential water-splitting photocatalyst. In addition, SiP_2 MLs have excellent electron mobility of 33,153 $cm^2 \cdot V^{-1} \cdot S^{-1}$. The calculated hydrogen adsorption free energy shows that SiP_2 ML possesses better HER ability compared to that of graphene.

Recently, Ren et al. [20] constructed different stacked $MoTe_2/PtS_2$ van der Waals heterostructures (vdWHs) and explored their electronic characteristics by using first-principles calculation. By changing stacking configurations, the $MoTe_2/PtS_2$ vdWHs could achieve a transition from type-I to type-II, which respectively possess potential applications in light emitting diode and photocatalysis. The type-II $MoTe_2/PtS_2$ vdWH has adequate band-edge alignment for overall water-splitting when pH is 0. In addition, $MoTe_2/PtS_2$ vdWHs possess excellent visible light absorption capacity. All the results show that $MoTe_2/PtS_2$ vdWHs are promising candidates as photocatalytic and photovoltaic devices.

We hope that this Special Issue of *Crystals*, entitled "Semiconductor Photocatalysts", will be able to provide assistance and guidance for the development and design of novel semiconductor photocatalysts.

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