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Enhancing the photocatalytic activity for pollutant degradation and H_2 evolution by modifying ZrO_2 with nanoclusters of $BiVO_3$, Ag_3PO_4, $SrTiO_3$ and WO_3: A first-principles study

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Environmental pollution and energy exhaustion has received much interest both in scientific and industrial research fields. For this reason, tremendous efforts are made to design novel environmentally friendly non-polluting and sustainable energy storage photocatalysts for efficient solar energy harvesting and conversion. Semiconductor-based photocatalysis has received increasing attention in energy storage and environmental remediation process due to the abundantly solar energy. For this purpose, several heterostructures using $BiVO_4$, Ag_3PO_4, $SrTiO_3$ and WO_3 monolayers coupled with ZrO_2 nano-cluster are designed to examine their potential applications in energy storage and degradation of pollutants using density functional theory calculations for the first time. Moreover, the underlying mechanism, band edge positions, optical and electronic properties of the ZrO_2-basedheterostructures are evaluated. The results displayed that the calculated band gap of the heterostructures is reduced compared to the pure ZrO_2, which favors redshift absorption. A type-I band alignment was attained for the $BiVO_4/ZrO_2$, Ag_3PO_4/ZrO_2 and WO_3/ZrO_2 heterostructures. More importantly, the type-II staggered band alignment formed in the $SrTiO_3/ZrO_2$ heterostructure restrained the charge recombination rate of the photoinduced carrier charges, as well as enhancing the photocatalytic activity. Our results display efficient charge separation and visible light response of the $BiVO_4/ZrO_2$, Ag_3PO_4/ZrO_2, WO_3/ZrO_2 and $SrTiO_3/ZrO_2$ heterostructures. In particular, suitable band alignment of $SrTiO_3/ZrO_2$ with enough driving forces for charge carrier transfer show overall water splitting and degradation of pollutant in which $SrTiO_3$ acted as the charge separation center. Thus, the $SrTiO_3/ZrO_2$ heterostructure emerges as a new type of ZrO_2-based photocatalyst for efficient solar energy applications. Furthermore, h+, HO• and O_2–• radicals played a major role in the photocatalysis process. Finally, possible charge separation and photocatalytic mechanisms of $BiVO_4/ZrO_2$, Ag_3PO_4/ZrO_2, WO_3/ZrO_2 and $SrTiO_3/ZrO_2$ heterostructures are proposed.

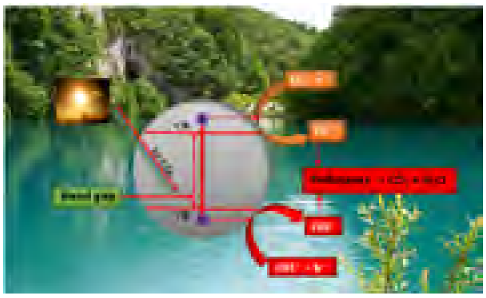

Figure 1: Schematic of the photodegradation mechanism of organic pollutants in water resources.

Biography

Francis Opoku received his BSc in Chemistry (2010) and MPhil in Inorganic Chemistry (2014) from the Kwame Nkrumah University of Science and Technology, Ghana. He is now pursuing PhD degree in Chemistry under the supervision of Dr. Penny Poomani Govender, Dr. Krishna Kuben Govender and Dr. Cornelia Gertina Catharina Elizabeth van Sittert in the Department of Applied Chemistry, University of Johannesburg, South Africa. His research interests include the design of efficient semiconductor-based photocatalyst materials and their applications in water splitting as well as degradation of pollutants in wastewater/water resources.

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