Theoretical investigation of Janus MoSSe/Ga2SSe heterostructures for photocatalytic applications

YANG Fan;[A] **RECORD Marie-Christine**;[A*] **BOULET Pascal**[A]

A) Aix-Marseille University, CNRS, IM2NP, 142 Av. Escadrille Normandie Niemen, Marseille, France

[*] m-c.record@univ-amu.fr

The two-dimensional Janus van der Waals heterojunctions, as novel asymmetric materials, have become highly promising photocatalysts due to their superior electronic structure and optical properties. In particular, the electronic properties of the type-2 band arrangement enable them to effectively separate photogenerated electrons and holes as Z-type photocatalysts,[1] and to transport the charge carriers along different pathways,[2] maintaining strong reduction and oxidation abilities, similar to green observations of plant photosynthesis.[3-5]

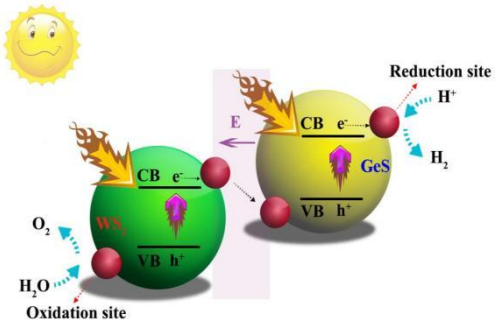

Figure 1. Principles of reactions of the direct Z-scheme system.[6]

In this work, we have systematically investigated the electronic structure and photocatalytic performance of MoSSe/Ga2SSe heterojunctions using density functional theory (DFT). Considering the interlayer van der Waals interaction, two exchange-correlation functionals (PBE and HSE06) have been used. By screening different interlayer distances and stacking patterns, multiple stable configurations have been ultimately obtained. Based on these stable configurations, the HSE06 functional appears to be superior to the PBE one with a more accurate bandgap. Subsequently, we have calculated with the HSE06 functional a series of properties, including band structures, density of states, electrostatic potentials, charge density differences, optical absorption coefficients. After analysis, these heterojunctions exhibit strong absorption performance in the visible and ultraviolet light ranges.

Keywords: heterojunctions; MoSSe/Ga2SSe; DFT.

[1] J.Li, Z.Zhang, W.Cui, et al. The spatially oriented charge flow and photocatalysis mechanism on internal van der Waals heterostructures enhanced g-C3N4. Acs Catalysis, 2018, 8(9): 8376-8385.

[2] S.A.Rawool, M.R.Pai, A.M.Banerjee, et al. pn Heterojunctions in NiO: TiO2 composites with type-II band alignment assisting sunlight driven photocatalytic H2 generation. Applied Catalysis B: Environmental, 2018, 221: 443-458.

[3] Q.Xu, L.Zhang, J.Yu, et al. Direct Z-scheme photocatalysts: Principles, synthesis, and applications. Materials Today, 2018, 21(10): 1042-1063.

[4] Z.Zhou, X.Niu, Y.Zhang, et al. Janus MoSSe/WSeTe heterostructures: a direct Z-scheme photocatalyst for hydrogen evolution. Journal of Materials Chemistry A, 2019, 7(38): 21835-21842.

[5] J.Yu, S.Wang, J.Low, et al. Enhanced photocatalytic performance of direct Z-scheme g-C3N4-TiO2 photocatalysts for the decomposition of formaldehyde in air. Physical Chemistry Chemical Physics, 2013, 15(39): 16883-16890.

[6] L.Ju, Y.Dai, W.Wei, et al. DFT investigation on two-dimensional GeS/WS2 van der Waals heterostructure for direct Z-scheme photocatalytic overall water splitting. Applied Surface Science, 2018, 434: 365-374.