

# 2D Heterostructures for Solar Energy Conversion: Role of Type-II and Z-scheme Charge Dynamics

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Abstract

The engineering of two-dimensional (2D) heterostructures represents a pivotal strategy in the development of sustainable energy technologies, particularly in the fields of photovoltaics and photocatalytic water splitting. Due to their exceptional electronic and optical properties, these materials provide an ideal platform for maximizing solar energy conversion and storage efficiency.

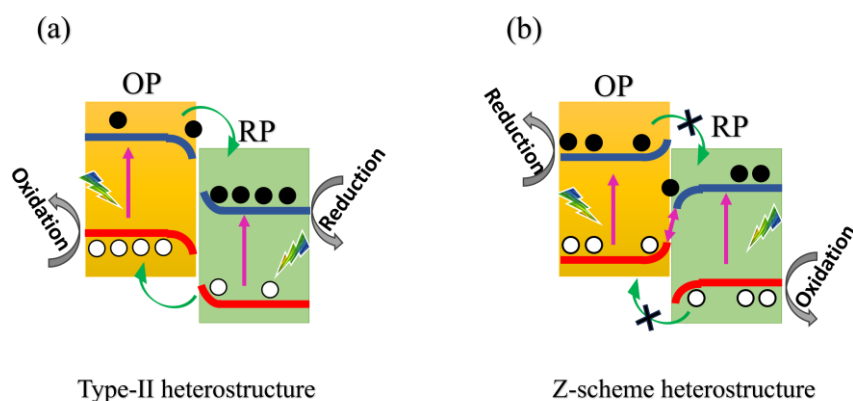
This work highlights the fundamental role of specific band alignment configurations—namely Type-II heterojunctions and Z-scheme systems in facilitating efficient charge separation and suppressing electron–hole recombination. In Type-II configurations, the spatial separation of e and h into distinct layers is crucial to reduce the recombination rate and therefore enhancing photocurrent in photovoltaic devices. On the other hand, the Z-scheme mechanism mimics natural photosynthesis to maintain high redox potentials, which is essential for driving the hydrogen evolution reaction in water splitting applications.

Drawing on recent literature and our previous findings, we showcase the potential of the novel InN/PtSSe heterostructure for highly efficient water splitting via a third-generation Z-scheme heterostructures [1]. Furthermore, we provide theoretical insights into the BAs/GeC van der Waals heterostructure, demonstrating how the Z-scheme architecture enables high-efficiency solar cell applications [2]. These results underscore the transformative potential of 2D heterostructures in designing high-performance, sustainable energy systems.

References

- [1] Chaoui, K., Hamidani, A., & Zanat, K. (2025). *International Journal of Hydrogen Energy*, 174, 151360.
- [2] Chaoui, K., Zanat, K., Elaggoune, W., Henrard, L., & Achehboune, M. (2024). *RSC advances*, 14(53), 39625-39635.

Figures



**Figure 1:** Comparative band alignment and carrier dynamics: Conventional Type-II vs. Z-scheme for water splitting and photovoltaics.