Piezoelectric-enhanced p-n junctions in photoelectrochemical systems

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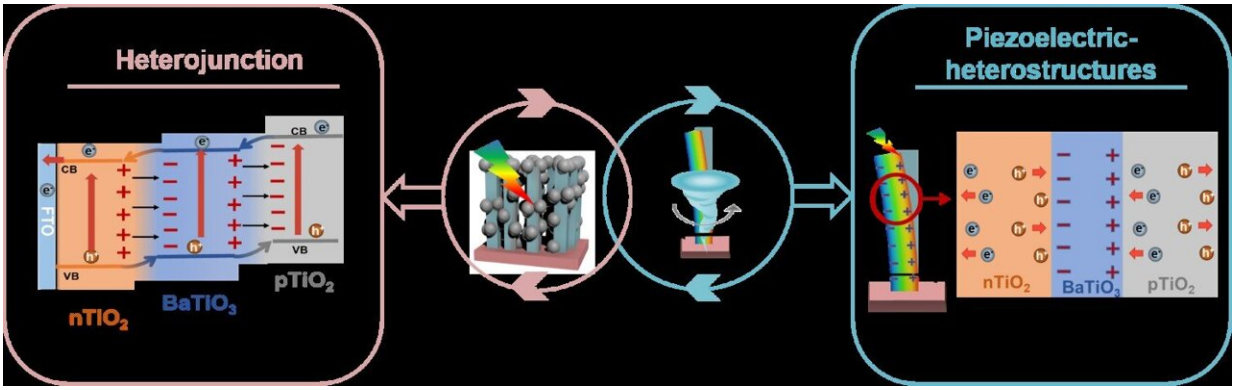

The formed built-in electric field and polarized-induced electric field at the interface of heterojunction to promote carrier separation. Credit: M. Ai et al

Photoelectrochemical (PEC) water splitting is a potentially feasible strategy for converting solar energy to green hydrogen. However, current PEC systems suffer from relatively low charge separation efficiency and sluggish water oxidation reaction, which prevent them from meeting the needs of practical applications. The main bottleneck like in achieving effective charge spatial separation, which is crucial for achieving efficient solar-to-hydrogen conversion.

Heterojunction engineering is one of the most promising methods for spatial charge separation, yet the carrier separation efficiency of heterojunction remains limited due to energy band matching or

interfacial and structural compatibility between different semiconductors. Meanwhile, the construction of p-n homojunction by finely controlling dopant or defect in semiconductors has been proven to be feasible, but the phenomenon that neutralizes the interfacial electric field through rapid accumulation of carriers during transfer process is largely negligible.

To that end, a team of researchers from the School of Chemical Engineering and Technology at Tianjin University, designed a unique n-TiO_2/$BaTiO_3$/p-TiO_2 heterojunction which couples with piezoelectric effect and p-n junctions to overcome the charge separation and transfer limitation of p-n junction.

"In our designed heterojunction, the ferroelectric $BaTiO_3$ layer is between n-TiO_2 with oxygen vacancies and p-TiO_2 with titanium vacancies," shares Minhua Ai, lead author of the study published in the journal *Green Energy & Environment*. "Consequently, the TBT3 achieves a prominent photocurrent density which is 2.4- and 1.5-times higher than TiO_2 and TiO_2–$BaTiO_3$ heterojunction, respectively."

Notably, driven by mechanical deformation, a stable polarized electric field formed in ferroelectric BaTiO3 can further regulate built-in electric fields based on comprehensive characterizations of charge carrier behaviors in such a multi-heterojunction. And n-TiO_2/$BaTiO_3$/p-TiO_2 heterojunction achieve piezoelectric-enhanced PEC performance (2.84 times higher than TiO_2 at 1.23 V vs. RHE).

"Based on the coupling with piezoelectric effect and p-n junctions, our work provides a piezoelectric polarization strategy for modulating the built-in electric field of heterojunction for charge separation enhancement," adds senior and corresponding author Lun Pan.

More information: Minhua Ai et al, Piezoelectric-enhanced n-

TiO2/BaTiO3/p-TiO2 heterojunction for highly efficient photoelectrocatalysis, *Green Energy & Environment* (2023). DOI: 10.1016/j.gee.2023.12.001