Efficient Photoconversion and Charge Separation of a (Mn^{2+}-Fe_2O_3)/RGO/(Fe^{3+}-WO_3) Photoelectrochemical Anode via Band-Structure Modulation

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We report on a (Mn2+-Fe2O3)/RGO/(Fe3+-WO3) hetero-nanostructure (HNS) as a building block for photoelectrochemical (PEC) anodes: an array of Fe3+-doped WO3 nanorods (NRs) were covered with RGO, and both the NRs and RGO were decorated with Mn2+-doped α-Fe2O3 nanoparticles (NPs). Efficient electron-hole separation and carrier migration are ascribed to mid-gap states (MGSs) obtained via doping, type-II band alignment of WO3 and α-Fe2O3, and highly conductive RGO. The optimum Mn2+ concentrations of 1% via experiment and 2% though density functional theory (DFT) are confirmed. DFT calculations reveal that the band structure of α-Fe2O3 can be modulated via tuning the Mn2+ concentration. With increasing Mn2+ concentration, the bandgap gradually narrows, and the MGSs gradually approach then merge into the valence band (VB) due to hybridization interactions between Mn2+, O2- and Fe3+ ions. Overall, we anticipate that this kind of HNS with modulated band structure can supply inspiration to the design and development of semiconductor materials for photoconversion applications.