Engineering Metal Halide Perovskite Heterojunction for Solar Fuel Production

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3D and 2D metal halide perovskites (MHPs) and perovskite derivatives have provoked a substantial revolution in the field of photovoltaics and optoelectronics because of their superior optical characteristics, physical properties' tunability, ease of fabrication, and low cost. In very recent times, MHPs have attracted a significant interest for their possible use in various photocatalytic applications. The suitability of MHPs in relevant solar-driven reactions comes essentially from their highly tunable and narrow band gap, long carrier lifetimes, and high mobilities, together with a good defect tolerance. In addition, their band alignment, relative to the potentials of common redox half-reactions, indicates the thermodynamic suitability of these materials to effectively run reduction reactions (H_2 generation, CO_2 reduction) and even oxidation reactions for MHPs with higher band gap values (e.g., chloride-based).[1] In this presentation, we will provide an overview of the research activity currently running in our research group aiming at exploiting the full potential of MHPs for solar fuel production. In particular, we will show how a rational materials chemistry engineering can be applied to modulate the photocatalytic properties for the intended solar-drive reaction. In addition, strategies to boost the activity through heterojunction design will be presented. Finally, through a combined experimental and computational modelling work details about the underlying mechanisms for hydrogen photogeneration and nitrogen fixation will be presented.[2–4]

References

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