The potential of 2D polymers for light harvesting applications

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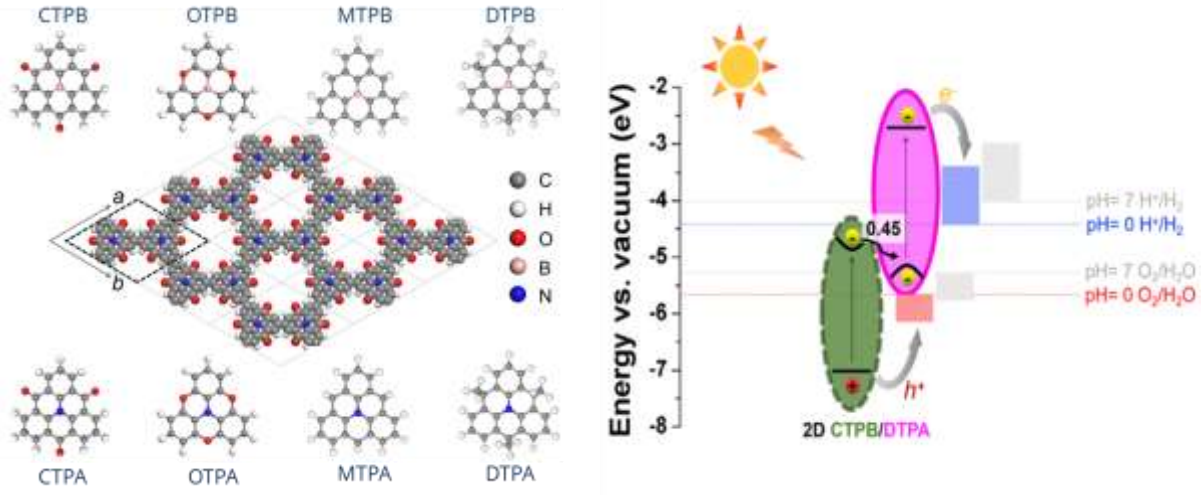
Decentralized production of green hydrogen by solar-fueled water splitting is key for a successful transfer to a zero emission energy supply. Our goal is the development of materials that are efficient photocatalysts without additional need for infrastructure, have long-term stability, and transform a considerable part of the solar spectrum to chemical and electric energy.

To achieve this goal we take advantage of various options that are offered by conjugated 2D polymers, in particular

- full conjugation to allow for band dispersion and high charge carrier mobility
- lattice symmetry that determines electronic band structure
- functionalization to in-plane control conjugation and photocatalytic performance
- functionalization with heteroatoms to shift bands with respect to vacuum

As example system we use honeycomb-kagome structures based on hetero-triangulenes [1,2]. If designed properly, they can be arranged in tandem cells where hydrogen and oxygen evolution is spatially separated, and no additional catalyst, voltage or sacrificial agent is required-(Figure) [3].



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[3] Y. Jing, Z. Zhou, W. Geng, X. Zhu, T. Heine, Adv. Mater. 33, 2008645 (2021).