Towards rational catalyst design?
Molecularly engineered frameworks for hydrogen evolution photocatalysis

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The conversion of sunlight into storable chemical fuels through photocatalysis has been identified as a viable strategy to alleviate future energy shortage. Although a number of potent semiconductors for solar water splitting are at hand, key features such as earth-abundance, stability and low toxicity still need to be addressed, thus calling for new material solutions for sustainable photocatalysis. While heterogeneous systems excel through their stability, homogeneous catalysts offer the potential to tune every step in the photocatalytic mechanism through molecular engineering. Combining the best of both worlds opens up new possibilities for the design of tailor-made photocatalysts.

We have recently developed a class of "soft" photocatalysts based on carbon nitrides and covalent organic frameworks (COFs),[1] which are abundant and molecularly tunable organic semiconductors. I will review our recent progress in the rational design of triazine- and heptazine-based systems for hydrogen evolution and highlight possible catalyst optimization strategies – through doping,[2] exfoliation,[3] functionalization,[4] and active site engineering,[5] as well as hybridization with bio-inspired co-catalysts.[6]

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