



DFT Assisted Predesign of Photocatalysts for Carbon Dioxide Reduction

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Features:

- Metal-Free
- Water as the reductant
- Low cost
- One pot
- High activity

Intro

Light-driven carbon dioxide reduction offers an economical solution to global warming and fuel production. But nowadays, most photocatalysts for carbon dioxide suffer from various disadvantages, like high cost or require additional reductants. Herein, we developed several kinds of photocatalysts for carbon dioxide reduction, which cost low and have relatively high performance. The best of our results reached over $100 \mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$ under visible light.

Predesign

- Select donor, acceptor, and linker;
- Structure optimization;
- Acquire molecular orbital information;
- Convert to RedOx potential;
- Evaluate photosensitivity.

Example

Donor: Triphenylamine
Acceptor: Triphenyltriazine
Linker: Azo
HOMO: -5.23 eV
LUMO: -2.63 eV
Band Gap: 2.60 eV
Wave length: 477 nm
Performance: $7 \mu\text{mol}\cdot\text{g}^{-1}\cdot\text{h}^{-1}$

Mechanism

