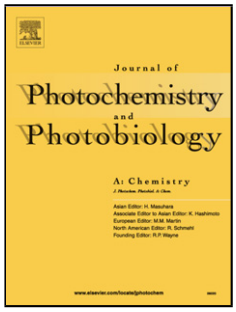

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Position of the Anchoring Group Determined the Sensitization Efficiency of Metal-Free D-π-A Dyes: Combined Experimental and TD–DFT Insights

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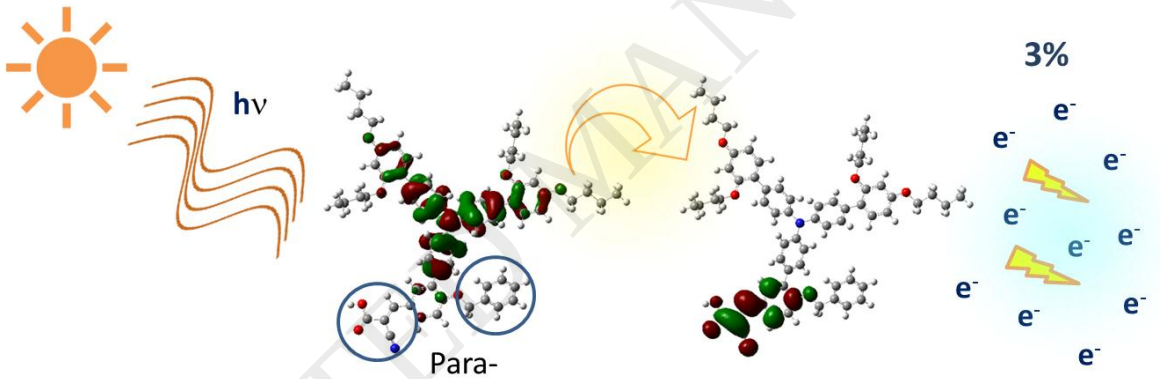
Graphical Abstract



Highlights

- Novel D-π-A organic sensitizers incorporating D35 as the electron donor were synthesized.
- The DFT calculations were successfully used to indicate the photosensitization properties.
- Electron delocalization on the dye molecule depends on the position of the anchoring group.
- The synthesized dyes have favorable band positions to the CB of TiO_2 and the redox potential of Co(II/III).
- The dye with the anchoring group in the para position has higher IPCE than that in the ortho position.

Abstract

We report on the design and synthesis of new D-π-A organic sensitizers incorporating D35 as the electron donor unit and (benzyloxy)benzene as the π- linker. The structure and yield of the