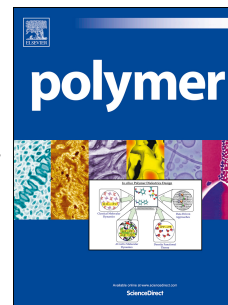


Accepted Manuscript

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PII: S0032-3861(17)30385-3

DOI: [10.1016/j.polymer.2017.04.017](https://doi.org/10.1016/j.polymer.2017.04.017)

Reference: JPOL 19597

To appear in: *Polymer*

Received Date: 9 January 2017

Revised Date: 3 April 2017

Accepted Date: 5 April 2017

Please cite this article as: Meier CB, Sprick RS, Monti A, Guiglion P, Lee J-SM, Zwijnenburg MA, Cooper AI, Structure-property relationships for covalent triazine-based frameworks: The effect of spacer length on photocatalytic hydrogen evolution from water, *Polymer* (2017), doi: 10.1016/j.polymer.2017.04.017.

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Structure-property relationships for covalent triazine-based frameworks: The effect of spacer length on photocatalytic hydrogen evolution from water

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Abstract:

Covalent triazine-based frameworks (CTFs) are a subclass of conjugated microporous polymers (CMPs) that can be used as organic photocatalysts for photocatalytic hydrogen evolution from water. Seven materials with varied spacer units from phenyl to quarterphenylene were synthesized, either by trifluoromethanesulfonic acid (TfOH) catalysis from nitriles or by Suzuki-Miyaura polycondensation. The photocatalytic performance under visible light of all materials was systematically studied in the presence of a hole-scavenger, showing that both synthesis routes produce CTFs with similar hydrogen evolution rates (HER), but different optical properties. The highest hydrogen evolution rate in the cyclotrimerized series was found for CTF-2 with an apparent quantum yield of 1.6% at 420 nm in a mixture of water and triethanolamine with a platinum co-catalyst. Based on (TD-)DFT calculations, the highest performance was expected for CTF-1 and this discrepancy is explained by a trade-off between increased light absorption and decreased thermodynamic driving force.

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