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Towards a greener synthesis of dibenzofuran based hole transporting materials (HTM) for perovskite solar cells

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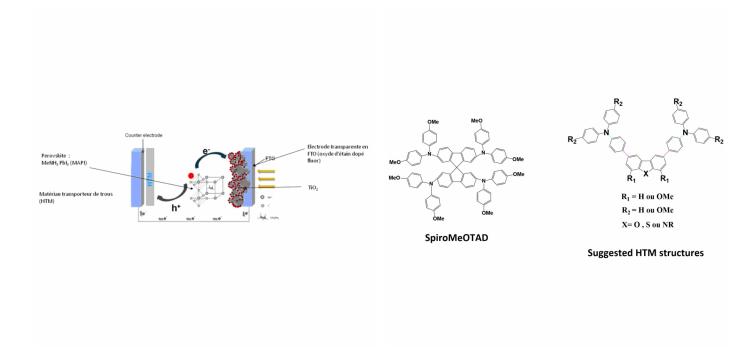
#### PURPOSE OF THE ABSTRACT

Solar power holds a promising future as a reliably available energy source and a remedy for the damage caused by fossil fuels. To harvest this energy, solar cells are used to absorb the light emitted from the sun and transform it into electrical energy. With efficiencies up to 25%,[1] perovskite solar cells need to be more accessible in terms of production (greener, more environmentally friendly) and usage. One of the obstacles blocking this accessibility is the synthesis process of the hole transporting materials (HTM), their stability, and production cost. In a perovskite solar cell (Figure 1), charge transfer occurs due to the generation of a hole/electron couple at the perovskite level, where the holes travel towards the HTM, and electrons towards the electrode. In a closed circuit, this leads to the flow of electric current.

SpiroMeOTAD is the most used HTM for perovskite solar cells.[2] It is a high-performing material, which comes at a high production cost, with complicated synthesis and purification steps, and lower cell stability (from the necessary doping it requires to function). We suggest a more environmentally compatible molecule (potentially bio-sourced) that has a lower production cost, easier synthesis, and purification, and which is potentially implementable without any doping (Figure 2).

Optimizing the synthesis step is necessary to lower the environmental impact of the HTM, with microwave-driven Suzuki reactions,[3] with lower metallic charges (from 5mol% to 1mol%), shorter reaction times (12h to 2h), and greener solvent. The main bio-sourced synthetic pathway (starting from guaiacol) will undergo the same optimization used in model reactions.

# **FIGURES**



## FIGURE 1

Figure 1

Composition of a perovskite solar cell

## FIGURE 2

Figure 2

Structure of the HTMs

### **KEYWORDS**

perovskite solar cells | nanocatalyst | hole transporting material | green synthesis

## **BIBLIOGRAPHY**

[1] Jeong, J., Kim, M., Seo, J. et al. Pseudo-halide anion engineering for alpha-FAPbl3 perovskite solar cells. Nature 2021, 592, 381–385. https://doi.org/10.1038/s41586-021-03406-5

[2] Gheno A., Vedraine S., Ratier B., Bouclé J. pi-Conjugated Materials as the Hole-Transporting Layer in Perovskite Solar Cells. Metals 2016, 6, 1-21. https://doi.org/10.3390/met6010021

[3] Iben Ayad A., Belda Marin C., et al. "Water soluble" palladium nanoparticle engineering for C–C coupling, reduction and cyclization catalysis. Green Chem. 2019, 21, 6646-6657. https://doi.org/10.1039/C9GC02546D