

Greener processability of PTAA based HTMs: Introducing Phenothiazine and Benzothiadiazole scaffolds to improve sustainability of flexible Perovskite Solar Cells

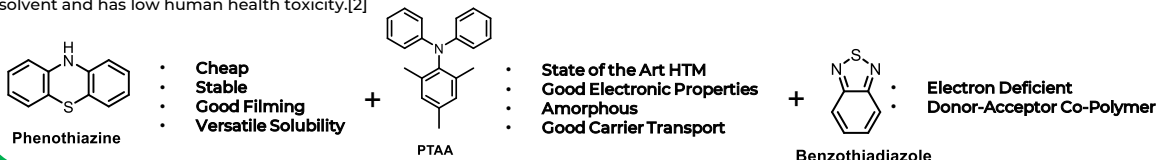
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Introduction

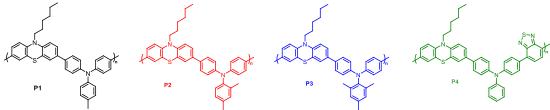
Recently, flexible Perovskite Solar Cells (f-PSC) have been a growing niche within the research on PSC with the aim of broadening its range of applications. However, to unlock f-PSC full potential, research must focus on boosting the performance, stability and sustainability, which can be achieved by working on the diverse device layers, among which Hole Transport Materials (HTMs) play a major role. State of the art polymeric HTMs, are still processed with toxic solvents such as chlorobenzene (CB), dichlorobenzene (DCB) or toluene[1], which pose an obvious barrier to the upscaling of this technology.

As the literature in green-solvent-deposition charge transport layers is still scarce, we present a new set of HTMs, based on different promising scaffolds, that are processed using Tetrahydrofuran (THF) that is non-aromatic, non-halogenated, cheap, a low environmental risk solvent and has low human health toxicity.[2]

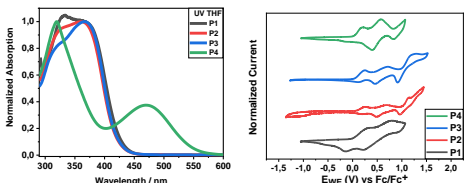


Results

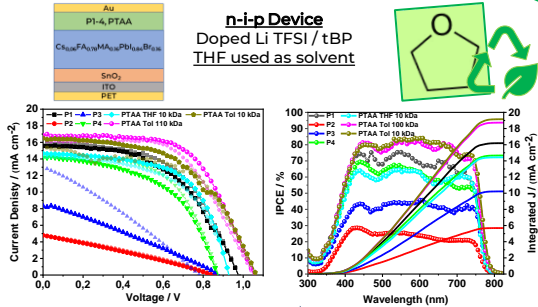
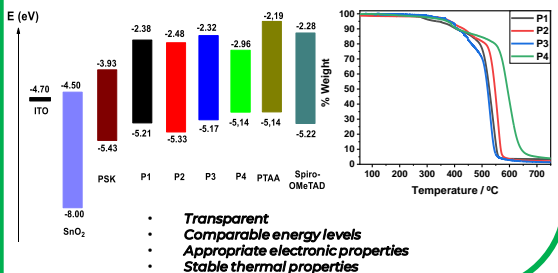
The novel HTMs incorporate additional scaffolds to the classic triphenylamine present in PTAA, with the scope of improving their solubility in THF. From which, the phenothiazine moiety was opted due to its good solubility in common organic solvents, high chemical stability, high hole mobilities and extremely low cost[3, 4]. The methyl substitution of the TPA phenyl unit was also altered to evaluate the trade-off effect on solubility and polymeric chain packing. Finally, we also considered the **benzothiadiazole unit** due to its functionalizable nature and electron deficient system[5], giving ability to tune the electronics of the system.



Characterisation



	$\lambda_{abs sol.}$ (nm)	E_g (eV)	E_{HOMO} (eV)	M_w (kDa)	DP	T_{stab} (°C)
P1	360	2,83	-5,21	12,6	1,37	337
P2	360	2,85	-5,33	18,3	1,46	384
P3	365	2,85	-5,17	12,6	1,37	374
P4	470	2,18	-5,14	19,2	1,11	373



Comparable Efficiencies to state of the Art PTAA in Toluene
Outperforming PTAA in THF

Conclusions

The novel polymers P1-4 were successfully synthesized using new protocols, adhering to Green Chemistry Principles[6], followed by a complete structural, optoelectronic, and thermal characterization.

P1-4 have appropriate band gaps and a HOMO band levels aligned with the valence band of perovskite. Additionally, they are thermally stable well above operating temperatures and withstand high annealing temperatures when applied for inverted structures.

P1-4 were implemented as HTMs on flexible n-i-p devices using PTAA as the reference. Results reveal that **P1** and **P4** can achieve competitive efficiencies compared to PTAA when processed with toluene, and even outperform it if processed with THF.

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