Supporting Information

Synthesis and Optical Characterisation of Triphenylamine-Based Hole Extractor Materials for CdSe Quantum Dots

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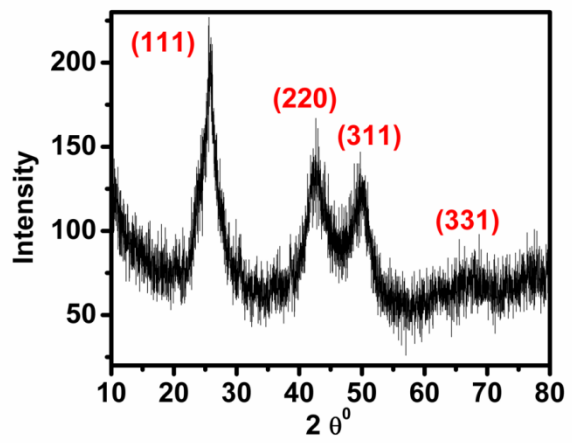

Figure S1. Powder X-Ray diffraction pattern of CdSe QDs. Lattice planes are marked.

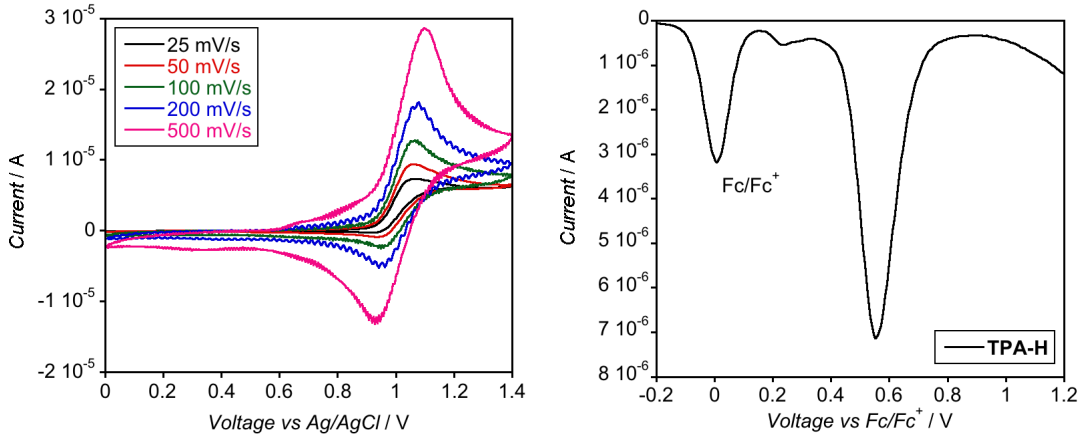

Figure S2. Cyclic voltammetry traces at different scan rates (*left*) and DPV scan (*right*) of **TPA-H**.

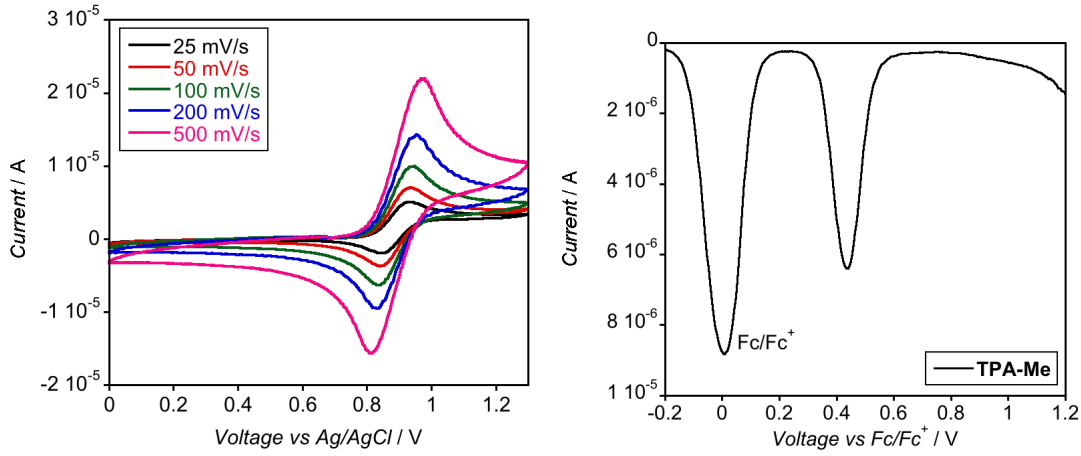

Figure S3. Cyclic voltammetry traces at different scan rates (*left*) and DPV scan (*right*) of **TPA-Me**.

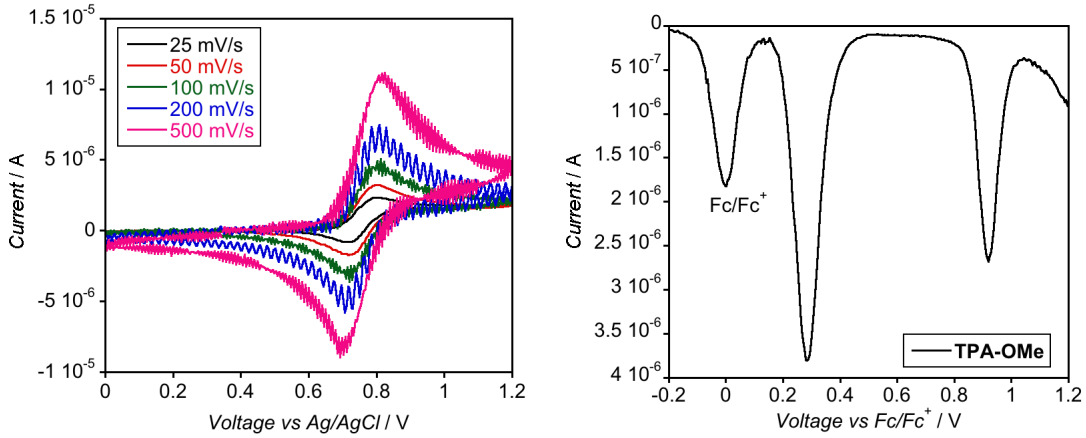

Figure S4. Cyclic voltammetry traces at different scan rates (*left*) and DPV scan (*right*) of **TPA-OMe**.

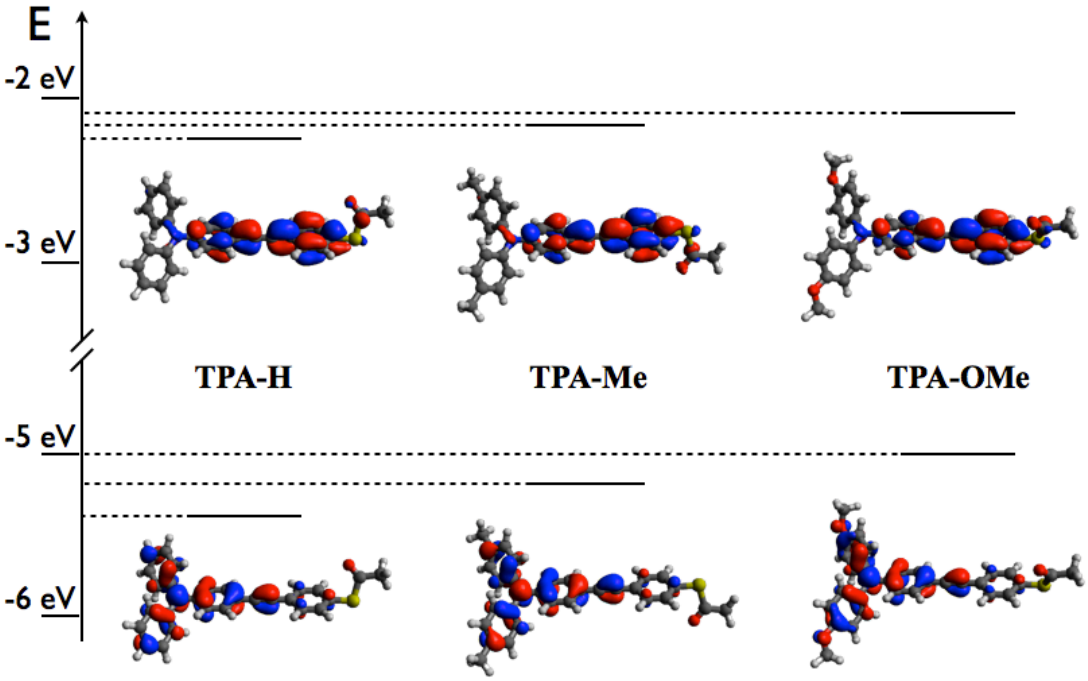

Figure S5. Molecular orbital distribution of HOMO (*bottom*) and LUMO (*top*) for TPA derivatives at B3LYP/6-31G(d) level of theory (isodensity = 0.03).

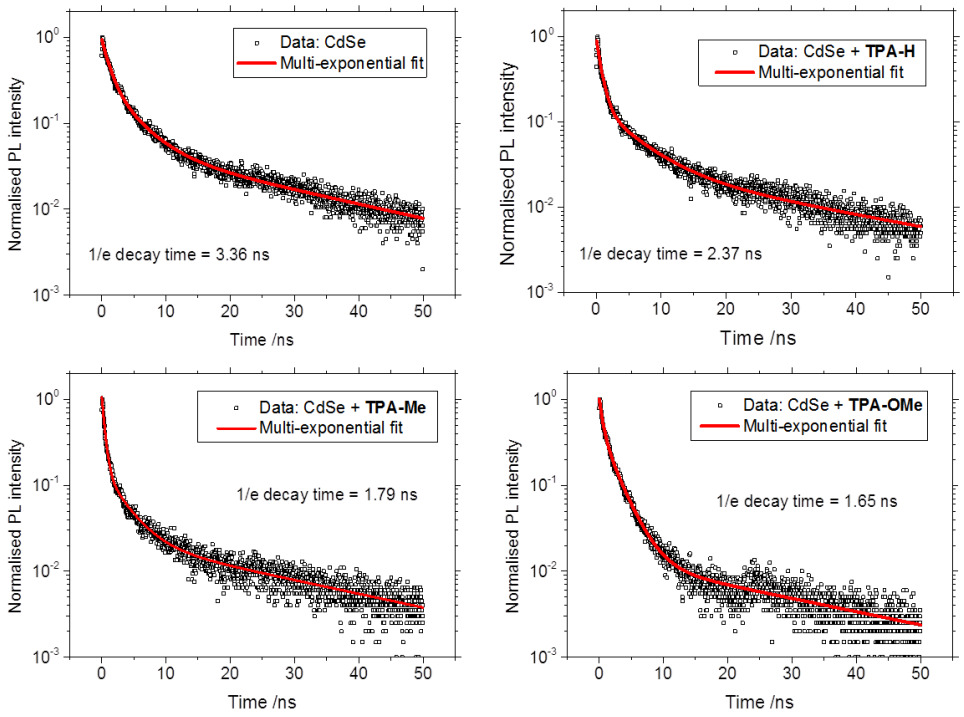

Figure S6. Multi (*tri*) exponential fits to the SPC data presented in Fig. 6 and the calculated 1/e decay times from each fit.

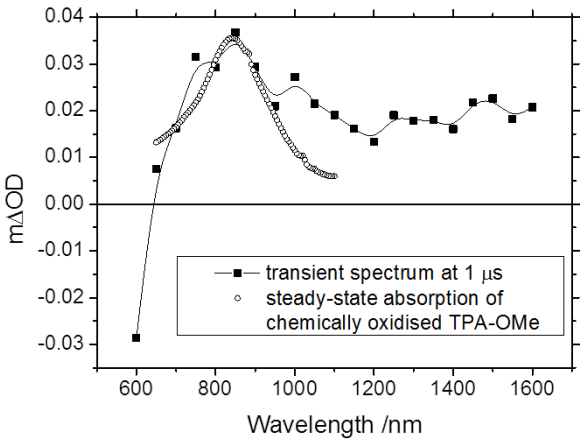

Figure S7. Transient absorption spectrum *(solid squares)* at 1 μs for the sample CdSe + **TPA-OMe**. Excitation was at 550 nm with an energy of 11.5 ± 1 μJ cm^{-2}. Overlaid *(open circles)* is the normalised steady-state absorption of chemically oxidised **TPA-OMe** in CH_2Cl_2.

2. Supporting Information Tables

Table S1. Total and reorganisation energies of TPA derivatives at B3LYP/6-31G(d) level of theory (C-PCM in toluene).[a]

	Energies / eV				
	E_0G_0	E_cG_0	E_0G_c	E_cG_c	**TPA → TPA$^+$** Reorg. energy
TPA-H	-39595.393024	-39589.998646	-39595.312885	-39590.075185	0.076539
TPA-Me	-41735.181770	-41729.900879	-41735.115777	-41729.966907	0.066028
TPA-OMe	-45828.041912	-45822.892667	-45827.951573	-45822.992373	0.099706

[a] E_0: Energy at the neutral state configuration (charge = 0, singlet); E_c: Energy at the cation configuration (charge = +1, doublet); G_0: Neutral state geometry; G_c: Cation geometry. Reorganisation energy after hole transfer = $E_cG_0 - E_cG_c$.