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Optimizing thienothiophene chain lengths of D-π-D hole transport materials in perovskite solar cells to improving energy levels and hole mobility

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Table S1 The calculated ionization potential, electron affinity, and fundamental gap of SS-2 – SS-6, unit in eV

Molecules	IP	EA	Fundamental gap
ss-2	4.46	1.78	2.68(2.71)
ss-3	4.47	1.87	2.60
ss-4	4.48	1.94	2.52
ss-5	4.49	2.01	2.48
ss-6	4.50	2.06	2.39

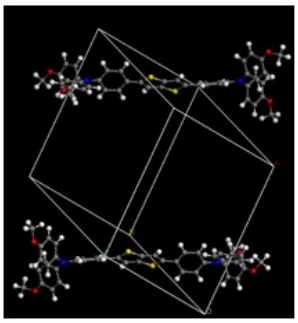
Table S2 Calculated maximum absorption wavelength (λmax, nm), maximum emission wavelengths(λ_{emi}, nm), stokes shift (nm), and main configurations.

Molecules	λ_{max}	Main configurations	λ_{em}	Stokes shift
ss-2	394(410)	H-L(89%)	492	98
ss-3	410	H-L(89%)	507	97
ss-4	422	H-L(87%)	519	97
ss-5	434	H-L(86%)	528	94
ss-6	444	H-L(85%)	534	90

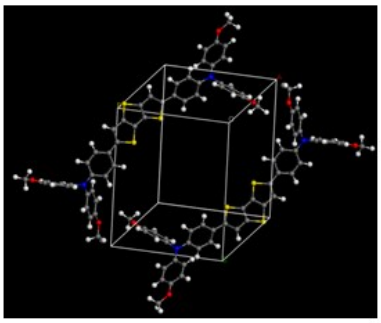
H denotes HOMO, L denotes LUMO

Table S3 Predicted crystal data of investigated molecules.

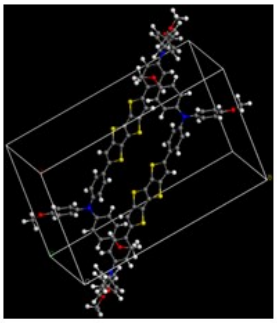
Molecules	Space group	ρ	Z	a	b	c	α	β	γ
SS-2	P1	1.219	2	17.00	14.16	12.11	52.10	86.92	66.50
SS-3	P1	1.287	2	11.75	12.31	14.69	90.25	102.12	94.43
SS-4	P1	1.269	2	13.76	23.83	9.46	100.68	51.49	82.01
SS-5	P1	1.302	2	13.04	15.05	12.38	85.83	102.60	99.91
SS-6	P1	1.305	2	15.35	20.94	14.79	48.45	44.05	62.30



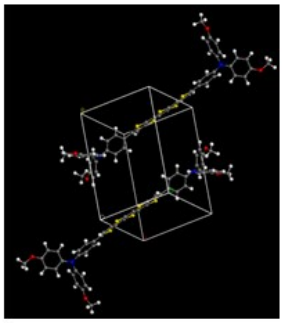
SS-2-crystal P1



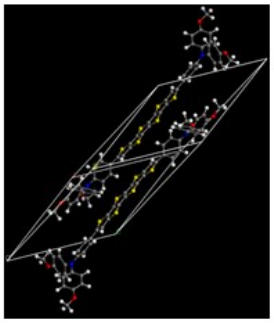
SS-3-crystal P1



SS-4-crystal P1



SS-5-crystal P1



SS-6-crystal P1

Figure S1 Predicted crystal structures of investigated molecules.