

Supplementary Table S2 Orbital contributions in dimers S₁–S₅ with different structures.

Excited state	MO	A		B		C		D		E		F	
		Hole contribution (%)	Electron contribution (%)	Hole contribution (%)	Electron contribution (%)	Hole contribution (%)	Electron contribution (%)	Hole contribution (%)	Electron contribution (%)	Hole contribution (%)	Electron contribution (%)	Hole contribution (%)	Electron contribution (%)
S ₁	HOMO	84.841	0.000	84.820	0.000	84.051	0.000	56.972	0.000	58.874	0.000	57.230	0.000
	LUMO	0.000	2.723	0.000	2.061	0.000	2.325	0.000	48.638	0.000	42.657	0.000	45.566
S ₂	HOMO	1.984	0.000	1.773	0.000	2.118	0.000	42.823	0.000	40.569	0.000	42.198	0.000
	LUMO	0.000	84.221	0.000	84.924	0.000	84.170	0.000	43.927	0.000	48.588	0.000	45.827
S ₃	HOMO	16.872	0.000	18.240	0.000	21.794	0.000	48.712	0.000	54.551	0.000	51.320	0.000
	LUMO	0.000	24.586	0.000	21.302	0.000	11.121	0.000	65.270	0.000	75.976	0.000	73.197
S ₄	HOMO	7.942	0.000	7.141	0.000	3.897	0.000	28.141	0.000	25.934	0.000	26.416	0.000
	LUMO	0.000	55.591	0.000	58.460	0.000	67.519	0.000	23.342	0.000	14.084	0.000	15.933
S ₅	HOMO	99.713	0.000	99.721	0.000	99.742	0.000	17.699	0.000	17.114	0.000	18.550	0.000
	LUMO	0.000	98.529	0.000	99.036	0.000	99.161	0.000	62.310	0.000	70.745	0.000	69.425