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Supporting information for

A theoretical study on a series of polycyclic conjugated hydrocarbons — dinaphthobenzo[1,2:4,5]dicyclobutadienes with the tunable charge transport property by controlling [N]phenylenes and (anti)aromaticity

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Section S.1. Computational Details of Marcus Rate Parameters.

Our simulation model is based on a combination of first-principles quantum mechanics calculations and Marcus semi-classical equation. By using the hopping mechanism to describe the charge transfer, the transfer rate (k) is described by the Marcus semi-classical equation:

$$k = \frac{V^2}{\hbar}\left(\frac{\pi}{\lambda k_B T}\right)^{1/2} \exp\left(-\frac{\lambda^2}{4k_B T}\right) \qquad (1)$$

Where V is the electronic coupling between adjacent molecules in the crystal structure, λ is the reorganization energy, T is the temperature and k_B is the Boltzmann constant.

The electronic coupling V of the two states (S_0 and S_n states) from the generalized Mulliken–Hush (GMH) formalism can be expressed as:

$$V = \frac{\mu_{tr}\Delta E}{\sqrt{(\Delta\mu)^2 + 4(\mu_{tr})^2}} \qquad (2)$$

Where μ_{tr} is the calculated transition dipole moment, $\Delta\mu$ is the dipole moment difference between S_0 and S_n states, which is negligible between two same molecules, and ΔE is the vertical excitation energy. The calculated values of V were summarized in Table S5, S8 and S9.

The λ of charge hopping depends on the rearrangement of the nuclear positions of molecules, we calculated λ as:

$$\lambda = \left[E^+(\mathrm{M}) - E^+(\mathrm{M}^+)\right] + \left[E(\mathrm{M}^+) - E(\mathrm{M})\right] \qquad (3)$$

Here, E(M) and E(M^+) are the neutral state energies at the optimal ground geometries and cation geometries, respectively. E^+(M^+) and E^+(M) refer to the energies of the cation state at the optimal cation and neutral geometries, respectively. The calculated values of λ were summarized in Table S6.

Based on these parameters, the charge hopping rate k can be obtained by Marcus semi-classical model. All the above mentioned calculations about Marcus rate expression were also performed in the Gaussian 16 A.03 software package.

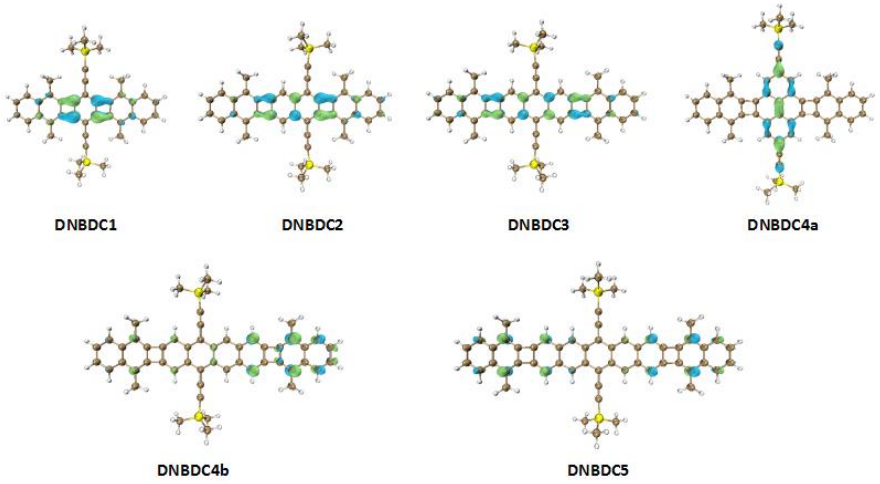

Figure S1. The LUMO+1 diagram for **DNBDC1~DNBDC5** at the MN15/6-31G* level.

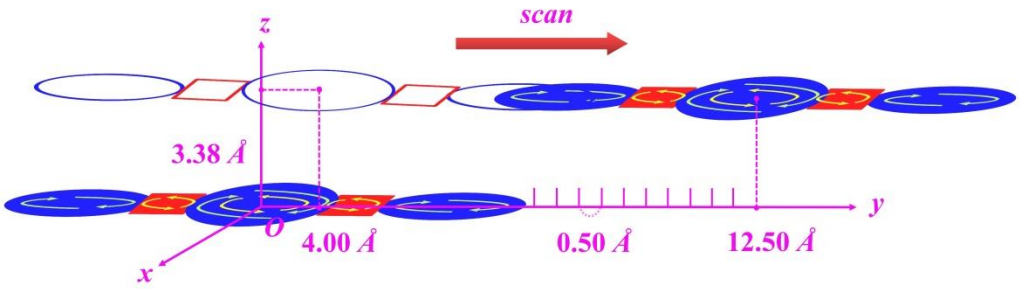

Figure S2. The schematic molecular packing model for DNBDCs (Herein, the centres of bottom DNBDC sets as the origin of coordinate, the direction of chain length sets as x-axis, the optimized step length of x-axis sets as 0.50 Å, the direction of chain wide sets as y-axis, and the direction of vertical interface packing sets as z-axis).

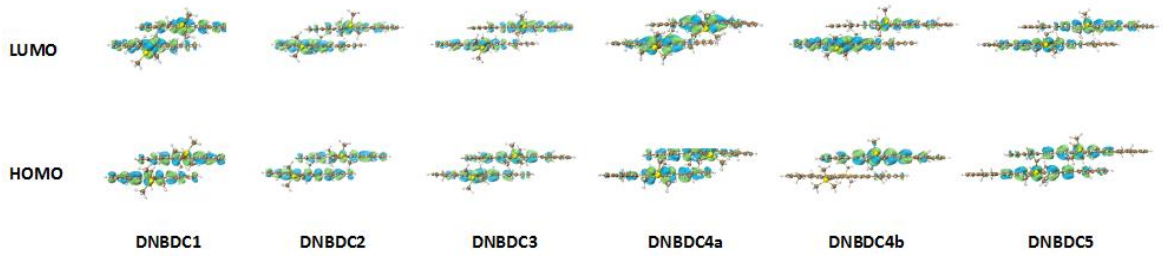

Figure S3. The FMO diagram for **DNBDC1~DNBDC5**-dimer at the *w*B97XD/6-31G* level.

Table S1. The experimental value and calculated frontier molecular orbitals (FMOs) for **DNBDC1** screened by different functionals (According to incremental HF exchange component (HF%)) at the 6-31G* basis set.

	HF%	HOMO	LUMO	E_g
exp.	--	-5.66	-2.96	2.70
B3LYP	0.20	-4.96	-1.98	2.97
B3PW91	0.20	-5.07	-2.10	2.97
PBE0	0.25	-4.41	-2.47	1.94
M06	0.27	-5.21	-1.89	3.32
PBE0-1/3	0.33	-4.41	-2.45	1.96
PBE38	0.38	-4.41	-2.44	1.97
MN15	0.44	-5.67	-1.46	4.20
M062X	0.54	-6.15	-1.33	4.83

Table S2. The calculated electron density (ED), Shannon entropy (SE) and shannon aromaticity (SA) values towards CBD1, CBD2 and core of **DNBDC1~ DNBDC5.**

	CBD1			CBD2			CORE		
	ED	SE	SA	ED	SE	SA	ED	SE	SA
DNBDC1	1.11	1.38	3.32×10^{-3}	1.11	1.38	3.33×10^{-3}	1.82	1.79	3.25×10^{-5}
DNBDC2	1.11	1.38	2.81×10^{-3}	1.11	1.38	3.03×10^{-3}	3.33	2.40	1.69×10^{-3}
DNBDC3	1.11	1.38	2.77×10^{-3}	1.11	1.38	2.33×10^{-3}	4.83	2.77	1.70×10^{-3}
DNBDC4a	1.12	1.38	6.92×10^{-3}	1.12	1.38	6.92×10^{-3}	5.75	2.94	8.88×10^{-4}
DNBDC4b	1.11	1.38	2.06×10^{-3}	1.10	1.38	1.88×10^{-3}	6.33	3.04	1.80×10^{-4}
DNBDC5	1.10	1.38	1.76×10^{-3}	1.10	1.38	1.76×10^{-3}	7.84	3.26	1.78×10^{-3}

Table S3. The optimized every step of the geometrical configuration for **DNBDC1-**dimer at CAM-B3LYP/6-31G* level.

x	HF(a.u.)	HF(eV)	Dipole (a.u.)		
			x	y	z
4.0	-4250.245635	-115653.43397399	-0.1064523	0.04449	0.1611256
4.5	-4250.249128	-115653.52902201	-0.0209489	0.0123234	-0.0004531
5.0	-4250.249167	-115653.53006963	0.0186209	-0.0083952	0.0044031
5.5	-4250.248963	-115653.52453764	-0.0281626	0.0019801	0.0240172
6.0	-4250.249122	-115653.52885330	-0.0163870	0.0084066	0.0066423
6.5	-4250.249085	-115653.52785466	-0.0370038	-0.002729	0.0191409
7.0	-4250.249108	-115653.52848867	0.0007372	-0.0004891	-0.0040644
7.5	-4250.249096	-115653.52814581	0.0003521	0.0081929	0.0084048
8.0	-4250.249107	-115653.52846146	0.0000979	-0.0000233	-0.0002703
8.5	-4250.246973	-115653.47038775	-0.0001228	0.0000164	0.0001402
9.0	-4250.246973	-115653.47038775	0.0000611	0.0000906	0.0002063
9.5	-4250.246981	-115653.47058639	-0.0030118	0.0009175	0.0008482
10.0	-4250.246213	-115653.44971283	0.0890626	-0.0368959	-0.0611204
10.5	-4250.246981	-115653.47058911	-0.0032691	0.0008801	0.0008255
11.0	-4250.244138	-115653.39325000	0.0133308	-0.0018121	-0.0109681
11.5	-4250.246725	-115653.46364214	0.2533142	0.0800023	-0.1160602
12.0	-4250.246866	-115653.46747073	-0.1891212	-0.0875232	0.0626859
12.5	-4250.247246	-115653.47781907	-0.4492933	-0.0431894	0.1640091

Table S4. The optimized every step of the geometrical configuration for **DNBDC1-**dimer at *w*B97XD/6-31G* level.

x	HF(a.u.)	HF(eV)	Dipole (a.u.)		
40	-4251.71706250	-115693.47298769	0.0031719	-0.0026329	-0.004768
45	-4251.71757180	-115693.48684625	0.0001558	-0.0000707	-0.0000724
50	-4251.71761670	-115693.48806802	-0.0003436	0.0001586	0.0007543
55	-4251.71761650	-115693.48806258	0.0001511	-0.0001881	-0.0005844
60	-4251.71761860	-115693.48811973	0.0000469	-0.0000021	-0.000087
65	-4251.71761840	-115693.48811428	0.0000470	0.0000342	0.0000628
70	-4251.71761800	-115693.48810340	-0.0000834	-0.00005	-0.000302
75	-4251.71761860	-115693.48811973	0.0000000	-0.0000946	-0.000151
80	-4251.71761860	-115693.48811973	0.0001811	-0.0000176	-0.0003315
85	-4251.71710840	-115693.47423667	0.0014098	-0.0016781	-0.0037522
90	-4251.71710860	-115693.47424212	-0.0014504	0.0017691	0.0037848
95	-4251.71710890	-115693.47425028	0.0018237	-0.0017798	-0.004057
100	-4251.71761840	-115693.48811428	-0.0001390	0.000009	0.0000824
105	-4251.71761930	-115693.48813877	0.0002342	-0.0001487	-0.0003806
110	-4251.71761880	-115693.48812517	-0.0000746	0.0000483	0.0000017
115	-4251.71694630	-115693.46982577	-0.0086917	0.0070095	-0.0193304
120	-4251.71761840	-115693.48811428	0.0001522	-0.0001454	-0.0003547
125	-4251.71693310	-115693.46946658	-0.0026414	0.0023603	-0.0311241

Table S5. The transition dipole moment of *x* (μ_x), *y* (μ_y) and *z* orientations (μ_z) (a.u.), the resultant transition dipole moment μ_{tr} (a.u.) and orbital energy difference ΔE (eV), and the electronic coupling values of each states *V* (eV), afterwards calculated the total electronic coupling values V_{total} (eV).

V-6.5 *Å*	States	μ_x	μ_y	μ_z	Dip.S	μ_{tr}	*OSC*	ΔE	*V*	V_{total}
DNBDC1	1	0.00	0.00	0.00	0.00	0.00	0.00	2.63	0.00	**4.00**
	2	-3.38	-0.27	-0.54	11.82	3.44	0.78	2.68	1.34	
	3	0.00	0.00	0.00	0.00	0.00	0.00	2.73	0.00	
	4	-0.06	0.23	-0.04	0.06	0.24	0.00	2.81	1.41	
	5	0.00	0.00	0.00	0.00	0.00	0.00	2.96	0.00	
	6	-0.54	-0.10	-0.46	0.51	0.72	0.04	2.99	1.49	
	7	-0.20	-0.07	-0.03	0.04	0.21	0.00	3.28	1.64	
	8	0.04	-0.21	0.04	0.05	0.22	0.00	3.33	1.67	
	9	0.00	0.00	0.00	0.00	0.00	0.00	3.36	0.00	
	10	0.00	0.00	0.00	0.00	0.00	0.00	3.38	0.00	
	11	-0.11	0.82	-0.03	0.68	0.82	0.06	3.47	1.74	
	12	0.00	0.00	0.00	0.00	0.00	0.00	3.48	0.00	
	13	0.00	0.00	0.00	0.00	0.00	0.00	3.49	0.00	
	14	3.15	0.11	0.25	9.96	3.16	0.90	3.67	1.83	
	15	0.00	0.00	0.00	0.00	0.00	0.00	3.72	0.00	
	16	1.49	0.16	0.07	2.26	1.50	0.21	3.73	1.86	
	17	0.00	0.00	0.00	0.00	0.00	0.00	3.77	0.00	
	18	2.12	0.28	0.54	4.86	2.21	0.45	3.77	1.88	
	19	0.42	-0.08	0.05	0.18	0.43	0.02	3.89	1.94	
	20	2.51	0.21	0.85	7.07	2.66	0.68	3.92	1.96	
DNBDC2	1	-2.26	0.34	-0.19	5.28	2.30	0.37	2.84	1.42	**4.30**
	2	3.13	0.22	0.40	10.02	3.16	0.70	2.84	1.42	
	3	-0.72	-0.47	-0.35	0.87	0.93	0.07	3.09	1.54	
	4	0.19	-0.20	0.09	0.08	0.29	0.01	3.16	1.58	
	5	0.14	-0.82	0.17	0.72	0.85	0.06	3.18	1.59	
	6	0.21	-0.05	0.09	0.06	0.23	0.00	3.28	1.64	
	7	-0.05	0.18	-0.25	0.10	0.32	0.01	3.34	1.67	
	8	0.09	-0.37	0.00	0.14	0.38	0.01	3.37	1.68	
	9	0.12	0.69	0.08	0.50	0.71	0.04	3.40	1.70	
	10	-0.52	0.29	0.09	0.37	0.61	0.03	3.45	1.73	
	11	0.10	0.10	-0.07	0.03	0.16	0.00	3.62	1.81	
	12	0.66	0.12	0.26	0.51	0.72	0.05	3.66	1.83	
	13	0.06	0.19	-0.10	0.05	0.23	0.00	3.68	1.84	
	14	-1.10	0.35	-0.15	1.35	1.16	0.12	3.71	1.86	
	15	-0.75	0.58	-0.11	0.91	0.95	0.08	3.74	1.87	
	16	-2.98	-0.23	-0.47	9.16	3.03	0.84	3.75	1.88	
	17	-4.24	0.00	-0.45	18.21	4.27	1.70	3.82	1.91	
	18	-0.64	0.25	-0.03	0.47	0.68	0.04	3.88	1.94	

	19	-1.03	-0.49	-0.11	1.32	1.15	0.13	3.93	1.96	
	20	-0.78	0.35	-0.36	0.86	0.93	0.08	3.96	1.98	
DNBDC3	1	-0.01	0.01	0.00	0.00	0.01	0.00	2.76	1.38	**3.79**
	2	0.53	-1.82	-0.01	3.59	1.89	0.25	2.79	1.40	
	3	4.17	0.23	-0.33	17.52	4.19	1.21	2.82	1.41	
	4	0.16	0.03	-0.01	0.03	0.16	0.00	2.83	1.41	
	5	-0.25	-0.14	0.19	0.12	0.34	0.01	2.94	1.47	
	6	0.01	0.00	0.00	0.00	0.00	0.00	2.99	0.00	
	7	0.00	-0.01	0.00	0.00	0.00	0.00	3.08	0.00	
	8	-0.42	0.06	0.52	0.45	0.67	0.03	3.14	1.57	
	9	0.28	0.54	-0.03	0.37	0.61	0.03	3.39	1.69	
	10	0.00	0.00	0.00	0.00	0.00	0.00	3.44	0.00	
	11	0.00	0.00	0.00	0.00	0.00	0.00	3.52	0.00	
	12	0.00	0.00	0.00	0.00	0.00	0.00	3.56	0.00	
	13	-0.13	-0.14	0.19	0.07	0.27	0.01	3.60	1.80	
	14	0.00	-0.01	0.00	0.00	0.00	0.00	3.64	0.00	
	15	0.51	-0.43	-0.12	0.46	0.68	0.04	3.66	1.83	
	16	0.07	-0.01	-0.01	0.01	0.07	0.00	3.67	1.83	
	17	2.78	-0.75	-0.35	8.41	2.90	0.76	3.68	1.84	
	18	6.57	0.68	-0.68	44.05	6.64	3.99	3.70	1.85	
	19	0.02	0.02	0.00	0.00	0.03	0.00	3.80	1.90	
	20	0.49	-1.63	-0.07	2.90	1.70	0.27	3.82	1.91	
DNBDC4a	1	0.00	-0.07	-0.01	0.00	0.07	0.00	2.53	1.26	**3.09**
	2	0.31	-1.59	0.07	2.61	1.62	0.17	2.60	1.30	
	3	0.11	-0.12	-0.01	0.03	0.16	0.00	2.68	1.34	
	4	0.22	-0.52	0.10	0.33	0.57	0.02	2.69	1.34	
	5	0.73	0.32	0.17	0.67	0.82	0.05	2.81	1.40	
	6	-0.16	-0.04	-0.02	0.03	0.17	0.00	2.82	1.41	
	7	1.92	0.15	0.23	3.75	1.94	0.26	2.85	1.42	
	8	-0.08	-0.01	-0.02	0.01	0.09	0.00	2.87	1.43	
	9	0.03	0.00	-0.01	0.00	0.04	0.00	3.20	1.60	
	10	0.04	-0.01	-0.01	0.00	0.04	0.00	3.25	1.62	
	11	-0.27	0.01	0.03	0.08	0.28	0.01	3.26	1.63	
	12	0.02	-0.01	-0.01	0.00	0.02	0.00	3.28	1.64	
	13	0.12	0.08	0.02	0.02	0.14	0.00	3.28	1.64	
	14	0.53	0.20	0.34	0.43	0.66	0.04	3.30	1.65	
	15	-1.57	-0.25	-0.15	2.55	1.60	0.21	3.38	1.69	
	16	-0.49	-0.06	-0.08	0.25	0.50	0.02	3.43	1.72	
	17	-3.78	-0.43	-0.55	14.81	3.85	1.25	3.44	1.72	
	18	-0.04	0.00	-0.01	0.00	0.04	0.00	3.44	1.72	
	19	-0.88	0.03	-0.25	0.85	0.92	0.07	3.60	1.80	
	20	0.06	0.00	0.00	0.00	0.06	0.00	3.64	1.82	
DNBDC4b	1	0.12	-1.72	0.00	2.97	1.72	0.17	2.34	1.17	**3.40**
	2	-0.16	-0.51	-0.01	0.29	0.54	0.02	2.35	1.18	
	3	-1.13	-0.31	0.07	1.39	1.18	0.09	2.52	1.26	

	4	0.52	-0.57	-0.05	0.60	0.77	0.04	2.54	1.27	
	5	-3.56	0.04	0.10	12.66	3.56	0.86	2.76	1.38	
	6	1.56	0.05	-0.01	2.45	1.56	0.17	2.78	1.39	
	7	0.27	0.29	-0.12	0.17	0.41	0.01	2.94	1.47	
	8	-0.94	-0.17	0.51	1.17	1.08	0.09	3.00	1.50	
	9	-0.42	0.32	0.32	0.38	0.61	0.03	3.06	1.53	
	10	0.08	-0.07	0.26	0.08	0.29	0.01	3.16	1.58	
	11	0.04	-0.28	0.03	0.08	0.28	0.01	3.28	1.64	
	12	-0.07	-0.15	-0.06	0.03	0.18	0.00	3.32	1.66	
	13	-0.13	-0.54	-0.04	0.30	0.55	0.03	3.36	1.68	
	14	-0.56	0.33	-0.11	0.44	0.66	0.04	3.43	1.71	
	15	-0.25	0.42	0.12	0.26	0.51	0.02	3.44	1.72	
	16	0.04	0.56	-0.07	0.32	0.56	0.03	3.46	1.73	
	17	2.33	-0.14	-0.16	5.46	2.34	0.47	3.51	1.75	
	18	-6.58	-0.04	0.50	43.48	6.59	3.77	3.54	1.77	
	19	0.56	0.68	-0.12	0.80	0.89	0.07	3.57	1.79	
	20	0.84	0.84	-0.09	1.42	1.19	0.13	3.61	1.80	
DNBDC5	1	-0.03	-0.61	-0.02	0.37	0.61	0.02	1.93	0.96	**2.60**
	2	-0.03	-1.83	0.06	3.37	1.84	0.16	1.93	0.97	
	3	0.06	0.20	0.02	0.04	0.21	0.00	2.15	1.07	
	4	0.40	0.79	0.06	0.79	0.89	0.04	2.17	1.09	
	5	3.69	-0.12	0.15	13.65	3.69	0.88	2.64	1.32	
	6	-0.90	0.01	-0.03	0.81	0.90	0.05	2.66	1.33	
	7	0.13	-0.01	0.00	0.02	0.13	0.00	2.77	1.39	
	8	0.77	-0.03	0.03	0.59	0.77	0.04	2.84	1.42	
	9	-1.34	0.04	0.18	1.82	1.35	0.13	2.85	1.43	
	10	1.62	0.04	-0.72	3.13	1.77	0.22	2.87	1.43	
	11	0.04	0.01	-0.04	0.00	0.06	0.00	2.95	1.47	
	12	0.00	0.25	0.10	0.07	0.26	0.01	2.98	1.49	
	13	0.04	0.00	0.01	0.00	0.05	0.00	3.09	1.54	
	14	0.55	-0.29	0.02	0.39	0.62	0.03	3.16	1.58	
	15	0.03	0.01	-0.01	0.00	0.03	0.00	3.19	1.60	
	16	0.59	0.22	0.19	0.43	0.66	0.03	3.30	1.65	
	17	-0.23	-0.04	-0.04	0.05	0.23	0.00	3.30	1.65	
	18	0.79	0.40	-0.13	0.80	0.90	0.07	3.33	1.67	
	19	0.16	0.07	-0.01	0.03	0.17	0.00	3.35	1.68	
	20	0.02	-0.03	0.03	0.00	0.05	0.00	3.38	1.69	

Table S6. The calculated reorganization energy λ(eV) for **DNBDC1~ DNBDC5.**

	E(M)	E(M^+)	E^+(M^+)	E^+(M)	EEP	EAV	λ
DNBDC1	-2123.88	-2123.92	-2123.92	-2123.88	0.04	0.03	0.24
DNBDC2	-2277.35	-2277.38	-2277.39	-2277.34	0.04	0.04	0.22
DNBDC3	-2430.80	-2430.84	-2430.85	-2430.80	0.05	0.04	0.22
DNBDC4a	-2506.93	-2506.97	-2506.97	-2506.92	0.05	0.04	0.24
DNBDC4b	-2584.25	-2584.31	-2584.31	-2584.25	0.06	0.05	0.21
DNBDC5	-2737.70	-2737.76	-2737.77	-2737.70	0.07	0.06	0.20

Table S7. The calculated charge hopping rates for **DNBDC1~ DNBDC5** at 6.5 *Å*, 8.5 *Å* and 14.9 *Å* by Marcus semi-classical equation.

		DNBDC1	**DNBDC2**	**DNBDC3**	**DNBDC4a**	**DNBDC4b**	**DNBDC5**
6.5 *Å*	k_1	5.45×10^{16}	7.86×10^{16}	6.20×10^{16}	3.34×10^{16}	5.42×10^{16}	3.54×10^{16}
8.5 *Å*	k_2	2.09×10^{16}	6.44×10^{16}	5.71×10^{16}	1.32×10^{16}	4.31×10^{16}	2.91×10^{16}
14.9 *Å*	k_3	6.14×10^{16}	1.03×10^{17}	1.05×10^{17}	3.18×10^{16}	7.31×10^{16}	4.00×10^{16}

Table S8. The transition dipole moment of *x* (μ_x), *y* (μ_y) and *z* orientations (μ_z) (a.u.), the resultant transition dipole moment μ_{tr} (a.u.) and orbital energy difference ΔE (eV), and the electronic coupling values of each states *V* (eV), afterwards calculated the total electronic coupling values V_{total} (eV) at 8.5 *Å*.

V_2-8.5 *Å*	*States*	μ_x	μ_y	μ_z	Dip.S	μ_{tr}	*OSC*	*E*	*V*	V_{total}
DNBDC1	1	-0.32	-1.52	0.04	2.40	1.55	0.08	1.31	0.66	**2.48**
	2	0.00	0.04	0.01	0.00	0.04	0.00	1.62	0.81	
	3	-0.01	0.02	0.00	0.00	0.02	0.00	1.87	0.93	
	4	0.01	0.06	-0.02	0.00	0.06	0.00	2.14	1.07	
	5	-0.17	1.35	0.02	1.86	1.36	0.10	2.19	1.10	
	6	0.05	0.03	0.00	0.00	0.06	0.00	2.42	1.21	
	7	-0.22	0.03	0.01	0.05	0.23	0.00	2.60	1.30	
	8	3.73	-0.20	-0.22	14.01	3.74	0.90	2.62	1.31	
	9	2.53	0.12	0.43	6.60	2.57	0.43	2.68	1.34	
	10	-0.69	0.03	-0.55	0.79	0.89	0.05	2.70	1.35	
	11	-0.12	0.07	0.00	0.02	0.14	0.00	2.75	1.37	
	12	0.16	-0.35	-0.28	0.22	0.47	0.02	2.76	1.38	
	13	-0.33	0.41	-0.05	0.28	0.53	0.02	2.90	1.45	
	14	-0.06	0.05	0.01	0.01	0.08	0.00	2.91	1.46	
	15	0.05	0.00	0.00	0.00	0.05	0.00	2.98	1.49	
	16	-0.26	-0.07	-0.02	0.07	0.27	0.01	3.07	1.53	
	17	-0.80	-0.30	-0.08	0.74	0.86	0.06	3.09	1.54	
	18	0.81	-0.09	0.05	0.67	0.82	0.05	3.11	1.56	
	19	-0.62	-0.50	-0.08	0.64	0.80	0.05	3.20	1.60	
	20	-3.74	-0.87	-0.29	14.83	3.85	1.18	3.26	1.63	
DNBDC2	1	-0.36	0.02	0.05	0.14	0.37	0.01	2.59	1.30	**3.90**
	2	-3.82	0.18	0.63	15.05	3.88	0.99	2.68	1.34	
	3	0.16	-0.44	-0.03	0.22	0.47	0.02	2.91	1.45	
	4	0.46	0.01	-0.06	0.21	0.46	0.02	2.95	1.48	
	5	-0.33	-0.03	0.04	0.11	0.33	0.01	2.97	1.48	
	6	0.16	0.87	-0.05	0.78	0.89	0.06	3.06	1.53	
	7	-0.03	-0.19	0.03	0.04	0.19	0.00	3.14	1.57	
	8	-0.23	-0.77	-0.03	0.65	0.81	0.05	3.19	1.59	
	9	-0.08	-0.58	0.07	0.35	0.59	0.03	3.20	1.60	
	10	-0.38	-0.60	0.02	0.50	0.71	0.04	3.37	1.69	
	11	-0.10	0.20	0.01	0.05	0.22	0.00	3.54	1.77	
	12	-0.49	-0.01	0.04	0.25	0.50	0.02	3.56	1.78	
	13	-1.29	0.03	0.16	1.70	1.30	0.15	3.62	1.81	
	14	-3.25	0.22	0.53	10.91	3.30	0.97	3.64	1.82	
	15	-0.45	-0.10	0.07	0.22	0.47	0.02	3.65	1.82	
	16	-5.16	0.24	0.73	27.27	5.22	2.46	3.68	1.84	
	17	1.41	-0.01	-0.22	2.02	1.42	0.18	3.70	1.85	
	18	0.53	0.21	-0.08	0.33	0.58	0.03	3.73	1.87	

	19	-0.83	-0.13	0.29	0.78	0.89	0.07	3.86	1.93	
	20	-0.38	0.44	0.20	0.38	0.62	0.04	3.89	1.94	
DNBDC3	1	-0.03	-1.58	0.01	2.49	1.58	0.15	2.51	1.26	**3.64**
	2	0.00	-0.02	0.00	0.00	0.02	0.00	2.56	1.28	
	3	-0.02	-0.01	-0.01	0.00	0.02	0.00	2.59	1.29	
	4	-4.13	0.04	0.61	17.41	4.17	1.16	2.72	1.36	
	5	0.03	0.28	0.00	0.08	0.28	0.01	2.83	1.41	
	6	0.10	1.03	-0.01	1.07	1.04	0.08	2.85	1.43	
	7	-0.40	0.04	-0.17	0.19	0.44	0.01	3.00	1.50	
	8	0.05	0.00	0.01	0.00	0.05	0.00	3.04	1.52	
	9	0.01	0.43	-0.01	0.19	0.43	0.02	3.34	1.67	
	10	-0.11	-0.38	0.02	0.16	0.40	0.01	3.39	1.70	
	11	-0.01	0.02	0.00	0.00	0.02	0.00	3.42	1.71	
	12	0.01	0.00	0.01	0.00	0.01	0.00	3.46	1.73	
	13	-0.08	-0.04	0.01	0.01	0.09	0.00	3.50	1.75	
	14	0.08	0.01	-0.01	0.01	0.08	0.00	3.51	1.76	
	15	-0.13	0.00	0.01	0.02	0.13	0.00	3.52	1.76	
	16	3.35	-0.04	-0.44	11.45	3.38	0.99	3.54	1.77	
	17	6.51	-0.03	-0.79	43.07	6.56	3.77	3.58	1.79	
	18	-0.28	0.03	0.04	0.08	0.28	0.01	3.60	1.80	
	19	0.00	0.68	0.00	0.46	0.68	0.04	3.72	1.86	
	20	-0.01	-1.57	0.01	2.45	1.57	0.22	3.73	1.86	
DNBDC4a	1	-0.26	-1.79	-0.02	3.28	1.81	0.05	0.68	0.34	**1.94**
	2	0.05	-0.48	-0.12	0.25	0.50	0.01	1.31	0.65	
	3	0.60	-0.22	0.31	0.50	0.71	0.02	1.36	0.68	
	4	-0.28	-0.06	0.00	0.08	0.29	0.00	1.70	0.85	
	5	-0.51	0.35	-0.16	0.41	0.64	0.02	1.81	0.91	
	6	-1.21	-0.12	-0.24	1.54	1.24	0.07	1.94	0.97	
	7	0.92	0.56	0.22	1.21	1.10	0.06	1.96	0.98	
	8	1.22	0.44	-0.08	1.70	1.30	0.09	2.11	1.05	
	9	0.51	0.72	0.10	0.78	0.88	0.04	2.26	1.13	
	10	0.55	-0.50	0.09	0.55	0.74	0.03	2.27	1.14	
	11	-1.14	0.44	0.01	1.49	1.22	0.09	2.34	1.17	
	12	0.34	1.03	0.05	1.18	1.09	0.07	2.42	1.21	
	13	-0.16	-0.37	-0.02	0.16	0.40	0.01	2.44	1.22	
	14	-0.11	-0.98	-0.17	1.00	1.00	0.06	2.48	1.24	
	15	0.26	0.22	-0.15	0.14	0.37	0.01	2.53	1.27	
	16	-0.27	-0.32	0.11	0.19	0.43	0.01	2.54	1.27	
	17	0.46	-0.13	0.03	0.23	0.48	0.01	2.60	1.30	
	18	-0.48	-1.73	-0.06	3.22	1.80	0.21	2.70	1.35	
	19	0.72	0.48	-0.31	0.85	0.92	0.06	2.75	1.38	
	20	-0.19	0.26	-0.12	0.12	0.34	0.01	2.80	1.40	
DNBDC4b	1	-0.11	1.41	0.00	1.99	1.41	0.09	1.83	0.91	**3.04**
	2	0.01	-0.18	0.01	0.03	0.18	0.00	2.05	1.03	
	3	0.03	0.14	-0.01	0.02	0.14	0.00	2.29	1.15	

	4	0.11	0.00	-0.08	0.02	0.13	0.00	2.36	1.18	
	5	-0.10	-1.33	-0.01	1.78	1.33	0.11	2.51	1.25	
	6	4.23	0.03	0.40	18.04	4.25	1.19	2.69	1.34	
	7	-0.47	-0.13	0.41	0.40	0.64	0.03	2.83	1.41	
	8	-0.13	-0.14	0.13	0.05	0.23	0.00	2.88	1.44	
	9	0.04	-0.07	-0.02	0.01	0.08	0.00	2.92	1.46	
	10	-0.08	0.14	-0.09	0.03	0.19	0.00	2.98	1.49	
	11	0.27	0.32	0.03	0.18	0.42	0.01	3.12	1.56	
	12	-0.26	0.41	-0.04	0.23	0.48	0.02	3.17	1.59	
	13	0.03	0.52	-0.03	0.27	0.52	0.02	3.19	1.60	
	14	-0.31	0.43	-0.01	0.28	0.53	0.02	3.25	1.62	
	15	0.05	-0.26	-0.06	0.07	0.27	0.01	3.30	1.65	
	16	-1.04	-0.08	-0.05	1.08	1.04	0.09	3.33	1.66	
	17	-0.11	0.04	0.02	0.01	0.11	0.00	3.39	1.69	
	18	-6.21	-0.05	-0.56	38.82	6.23	3.24	3.40	1.70	
	19	1.78	-0.64	0.19	3.59	1.89	0.30	3.43	1.71	
	20	-2.39	-1.00	-0.16	6.75	2.60	0.58	3.48	1.74	
DNBDC5	1	-0.32	-1.52	0.04	2.40	1.55	0.08	1.31	0.66	**2.36**
	2	0.00	0.04	0.01	0.00	0.04	0.00	1.62	0.81	
	3	-0.01	0.02	0.00	0.00	0.02	0.00	1.87	0.93	
	4	0.01	0.06	-0.02	0.00	0.06	0.00	2.14	1.07	
	5	-0.17	1.35	0.02	1.86	1.36	0.10	2.19	1.10	
	6	0.05	0.03	0.00	0.00	0.06	0.00	2.42	1.21	
	7	-0.22	0.03	0.01	0.05	0.23	0.00	2.60	1.30	
	8	3.73	-0.20	-0.22	14.01	3.74	0.90	2.62	1.31	
	9	2.53	0.12	0.43	6.60	2.57	0.43	2.68	1.34	
	10	-0.69	0.03	-0.55	0.79	0.89	0.05	2.70	1.35	
	11	-0.12	0.07	0.00	0.02	0.14	0.00	2.75	1.37	
	12	0.16	-0.35	-0.28	0.22	0.47	0.02	2.76	1.38	
	13	-0.33	0.41	-0.05	0.28	0.53	0.02	2.90	1.45	
	14	-0.06	0.05	0.01	0.01	0.08	0.00	2.91	1.46	
	15	0.05	0.00	0.00	0.00	0.05	0.00	2.98	1.49	
	16	-0.26	-0.07	-0.02	0.07	0.27	0.01	3.07	1.53	
	17	-0.80	-0.30	-0.08	0.74	0.86	0.06	3.09	1.54	
	18	0.81	-0.09	0.05	0.67	0.82	0.05	3.11	1.56	
	19	-0.62	-0.50	-0.08	0.64	0.80	0.05	3.20	1.60	
	20	-3.74	-0.87	-0.29	14.83	3.85	1.18	3.26	1.63	

Table S9. The transition dipole moment of *x* (μ_x), *y* (μ_y) and *z* orientations (μ_z) (a.u.), the resultant transition dipole moment μ_{tr} (a.u.) and orbital energy difference ΔE (eV), and the electronic coupling values of each states *V* (eV), afterwards calculated the total electronic coupling values V_{total} (eV) at 14.9 *Å*.

V_3-14.9 *Å*	*States*	μ_x	μ_y	μ_z	Dip.S	μ_{tr}	*OSC*	*E*	*V*	V_{total}
DNBDC1	1	-3.58	1.70	0.42	15.87	3.98	1.06	2.73	1.37	**4.25**
	2	0.00	0.00	0.00	0.00	0.00	0.00	2.75	0.00	
	3	0.06	0.12	-0.01	0.02	0.14	0.00	2.80	1.40	
	4	0.12	0.26	-0.01	0.08	0.28	0.01	2.80	1.40	
	5	0.54	0.79	-0.07	0.91	0.96	0.08	3.52	1.76	
	6	-0.15	-0.23	0.02	0.08	0.28	0.01	3.52	1.76	
	7	-5.06	2.32	0.58	31.31	5.60	2.87	3.75	1.87	
	8	-0.09	0.04	0.01	0.01	0.10	0.00	3.76	1.88	
	9	-1.55	0.70	0.18	2.93	1.71	0.27	3.76	1.88	
	10	-0.07	0.03	0.01	0.01	0.07	0.00	3.79	1.89	
	11	-0.03	0.03	0.00	0.00	0.04	0.00	3.79	1.90	
	12	0.13	-0.07	-0.02	0.02	0.15	0.00	3.79	1.90	
	13	-0.10	0.06	0.02	0.01	0.12	0.00	3.96	1.98	
	14	0.00	0.01	0.00	0.00	0.00	0.00	3.96	0.00	
	15	0.00	0.00	0.00	0.00	0.00	0.00	3.97	0.00	
	16	-0.01	0.00	0.00	0.00	0.01	0.00	3.98	1.99	
	17	0.05	0.01	-0.03	0.00	0.06	0.00	4.26	2.13	
	18	-1.33	-0.67	0.13	2.23	1.49	0.23	4.27	2.14	
	19	2.29	-0.55	-0.28	5.62	2.37	0.59	4.28	2.14	
	20	0.00	-0.05	-0.01	0.00	0.05	0.00	4.28	2.14	
DNBDC2	1	3.85	-1.56	-0.38	17.40	4.17	1.15	2.70	1.35	**4.92**
	2	0.44	-0.21	-0.07	0.24	0.49	0.02	2.72	1.36	
	3	-0.23	-0.42	0.03	0.23	0.48	0.02	2.97	1.49	
	4	0.19	0.36	-0.04	0.17	0.41	0.01	2.98	1.49	
	5	-0.64	-1.01	0.11	1.43	1.20	0.11	3.17	1.59	
	6	0.42	0.84	-0.09	0.88	0.94	0.07	3.17	1.59	
	7	-1.39	0.47	0.11	2.16	1.47	0.19	3.63	1.82	
	8	-0.70	0.33	0.08	0.60	0.77	0.05	3.65	1.82	
	9	6.59	-2.49	-0.65	50.03	7.07	4.51	3.68	1.84	
	10	-1.40	0.60	0.12	2.34	1.53	0.21	3.71	1.86	
	11	1.18	-0.37	-0.14	1.56	1.25	0.14	3.72	1.86	
	12	-0.49	0.28	0.08	0.33	0.57	0.03	3.73	1.87	
	13	-0.20	0.15	0.03	0.06	0.25	0.01	3.76	1.88	
	14	-0.22	0.13	0.04	0.07	0.26	0.01	3.90	1.95	
	15	-0.17	0.02	0.05	0.03	0.17	0.00	3.91	1.96	
	16	0.03	-0.23	0.00	0.05	0.23	0.01	3.92	1.96	
	17	-0.62	-1.54	0.09	2.75	1.66	0.27	4.03	2.01	

	18	0.77	0.91	-0.12	1.44	1.20	0.14	4.04	2.02	
	19	-0.97	-1.38	0.15	2.87	1.69	0.29	4.06	2.03	
	20	1.79	-1.43	-0.15	5.25	2.29	0.52	4.07	2.04	
DNBDC3	1	0.43	0.74	0.10	0.74	0.86	0.05	2.59	1.30	**4.05**
	2	-1.01	-1.69	-0.23	3.94	1.98	0.25	2.60	1.30	
	3	-4.41	1.39	-0.37	21.50	4.64	1.44	2.73	1.37	
	4	0.16	-0.05	0.02	0.03	0.17	0.00	2.75	1.38	
	5	1.28	0.05	0.09	1.64	1.28	0.14	3.48	1.74	
	6	-1.05	0.01	-0.08	1.10	1.05	0.09	3.50	1.75	
	7	0.94	0.20	0.12	0.94	0.97	0.08	3.51	1.76	
	8	0.98	0.28	0.13	1.06	1.03	0.09	3.52	1.76	
	9	-0.38	0.12	-0.03	0.16	0.40	0.01	3.53	1.77	
	10	-1.07	0.45	-0.12	1.36	1.17	0.12	3.54	1.77	
	11	-3.52	1.03	-0.28	13.50	3.67	1.17	3.55	1.78	
	12	0.28	-0.03	0.03	0.08	0.28	0.01	3.56	1.78	
	13	7.35	-1.97	0.66	58.29	7.63	5.13	3.59	1.79	
	14	-0.01	-0.01	-0.01	0.00	0.02	0.00	3.65	1.82	
	15	-0.90	2.05	0.00	4.99	2.23	0.46	3.73	1.86	
	16	0.15	-0.57	-0.02	0.35	0.59	0.03	3.73	1.86	
	17	0.16	0.50	0.06	0.28	0.53	0.03	3.76	1.88	
	18	0.25	0.20	0.05	0.10	0.32	0.01	3.78	1.89	
	19	-0.07	0.08	-0.01	0.01	0.11	0.00	3.84	1.92	
	20	0.00	-0.09	0.00	0.01	0.09	0.00	3.84	1.92	
DNBDC4a	1	0.05	-0.08	0.00	0.01	0.09	0.00	2.23	1.12	**3.01**
	2	1.18	-1.72	0.10	4.33	2.08	0.24	2.23	1.12	
	3	0.07	-0.13	0.00	0.02	0.14	0.00	2.27	1.14	
	4	0.12	-0.12	0.01	0.03	0.17	0.00	2.27	1.14	
	5	-2.01	-0.92	-0.20	4.91	2.22	0.33	2.73	1.37	
	6	-0.06	-0.03	0.00	0.00	0.06	0.00	2.74	1.37	
	7	-0.02	0.01	0.00	0.00	0.02	0.00	2.78	1.39	
	8	0.00	0.00	0.00	0.00	0.00	0.00	2.78	0.00	
	9	-0.08	-0.02	0.00	0.01	0.08	0.00	3.16	1.58	
	10	0.09	0.05	0.02	0.01	0.10	0.00	3.16	1.58	
	11	0.39	-0.29	0.04	0.24	0.49	0.02	3.19	1.60	
	12	0.32	-0.21	0.03	0.15	0.39	0.01	3.20	1.60	
	13	-4.24	-1.90	-0.42	21.78	4.67	1.73	3.25	1.63	
	14	-0.12	-0.05	-0.01	0.02	0.13	0.00	3.28	1.64	
	15	0.07	0.03	0.01	0.01	0.08	0.00	3.29	1.65	
	16	0.17	0.10	0.03	0.04	0.20	0.00	3.33	1.66	
	17	-0.04	0.01	0.04	0.00	0.06	0.00	3.50	1.75	
	18	0.16	-0.04	0.01	0.03	0.16	0.00	3.51	1.75	
	19	-2.60	-1.12	-0.26	8.06	2.84	0.72	3.64	1.82	
	20	-0.46	-0.20	-0.05	0.26	0.51	0.02	3.65	1.82	
DNBDC4b	1	-1.98	0.45	0.05	4.13	2.03	0.06	0.56	0.28	**3.95**
	2	0.01	-0.92	-0.14	0.87	0.93	0.01	0.60	0.30	

	3	-2.72	0.14	0.02	7.40	2.72	0.26	1.45	0.73	
	4	0.33	-0.07	-0.12	0.13	0.36	0.01	1.61	0.81	
	5	0.32	-0.17	-0.02	0.13	0.36	0.01	2.00	1.00	
	6	-1.27	0.23	-0.04	1.68	1.30	0.09	2.07	1.04	
	7	-1.52	0.94	-0.09	3.21	1.79	0.17	2.11	1.06	
	8	0.97	-0.18	0.01	0.98	0.99	0.05	2.17	1.09	
	9	-0.33	-1.80	0.21	3.39	1.84	0.18	2.19	1.10	
	10	0.54	0.44	0.06	0.49	0.70	0.03	2.47	1.24	
	11	-0.21	-0.08	0.08	0.06	0.24	0.00	2.53	1.27	
	12	-0.17	0.01	0.01	0.03	0.18	0.00	2.64	1.32	
	13	-2.70	-1.05	-0.17	8.42	2.90	0.56	2.70	1.35	
	14	3.13	0.97	0.10	10.73	3.28	0.72	2.75	1.37	
	15	2.74	0.72	0.05	8.02	2.83	0.55	2.81	1.40	
	16	3.18	1.22	0.00	11.60	3.41	0.83	2.92	1.46	
	17	-0.42	-0.32	-0.03	0.28	0.53	0.02	3.08	1.54	
	18	-0.53	0.03	0.00	0.28	0.53	0.02	3.11	1.56	
	19	2.72	0.26	0.00	7.46	2.73	0.58	3.15	1.57	
	20	0.51	1.14	0.23	1.61	1.27	0.12	3.16	1.58	
DNBDC5	1	2.03	0.59	0.11	4.48	2.12	0.05	0.47	0.23	**2.77**
	2	1.83	-0.54	-0.05	3.66	1.91	0.06	0.72	0.36	
	3	-0.24	0.40	0.03	0.22	0.47	0.01	1.09	0.54	
	4	1.52	-1.10	0.05	3.53	1.88	0.13	1.53	0.76	
	5	1.15	1.74	-0.14	4.37	2.09	0.18	1.68	0.84	
	6	2.97	0.50	-0.11	9.07	3.01	0.41	1.83	0.92	
	7	-0.56	-0.05	0.06	0.32	0.57	0.02	1.94	0.97	
	8	-0.63	-0.15	0.01	0.42	0.65	0.02	2.01	1.01	
	9	-0.06	-0.12	-0.05	0.02	0.14	0.00	2.27	1.14	
	10	0.04	-0.09	-0.02	0.01	0.10	0.00	2.36	1.18	
	11	0.88	-0.26	0.00	0.85	0.92	0.05	2.47	1.23	
	12	0.13	-0.18	-0.04	0.05	0.22	0.00	2.54	1.27	
	13	3.70	-0.68	-0.19	14.21	3.77	0.90	2.58	1.29	
	14	0.51	-0.07	0.01	0.26	0.51	0.02	2.68	1.34	
	15	-0.30	-0.24	-0.01	0.15	0.38	0.01	2.69	1.35	
	16	4.25	-1.18	-0.02	19.45	4.41	1.31	2.75	1.37	
	17	-1.56	0.53	0.13	2.73	1.65	0.19	2.81	1.40	
	18	-0.95	0.28	0.01	0.99	0.99	0.07	2.93	1.46	
	19	-0.42	0.46	-0.04	0.39	0.62	0.03	2.93	1.47	
	20	-0.63	-0.35	-0.01	0.52	0.72	0.04	2.96	1.48	