Supporting Information

Computational Investigation of Charge Injection, and Transport Properties of a Series of Thiophene—pyrrole–based Oligo-azomethines

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TABLE S1: IP(v,a)s and EA(v,a)s of all the studied compounds calculated at B3LYP/6-31G(d,p) level of theory. All energies are in eV.

		1	2	3	4	5	6	7	8
IP(a)	1	6.6183	6.5180	6.9466	6.3213	6.2057	7.1892	6.4701	5.9212
	2	5.7366	5.6206	6.1559	5.6323	5.3146	6.4641	5.4264	4.9817
	3	5.3744	5.2433	5.8430	5.3740	4.9509	6.1814	5.0472	4.5858
	4	5.1848	5.0610	5.6853	5.2497	4.7100	6.0379	4.8139	4.3715
	5	5.0700	4.9452	5.5893	5.1745	4.6792	5.9471	4.6915	4.2406
IP(v)	1	6.8154	6.7095	7.1759	6.5196	6.4542	7.4067	6.6665	6.1482
	2	5.9012	5.7887	6.3629	5.8830	5.5653	6.6462	5.5801	5.1499
	3	5.5190	5.3986	6.0178	5.6145	5.1658	6.3326	5.1809	4.7341
	4	5.3126	5.1998	5.8328	5.4681	4.9550	6.1588	4.9334	4.5039
	5	5.1812	5.0644	5.7088	5.3617	4.7962	6.0446	4.7970	4.3590
EA(a)	1	0.0551	0.0514	0.4217	0.0525	0.0187	0.7835	0.0991	-0.0475
	2	1.0262	0.9945	1.3786	0.8227	0.9571	1.7339	0.9892	0.7634
	3	1.4391	1.4139	1.7617	1.1328	1.3883	2.0955	1.3719	1.1102
	4	1.6641	1.6150	1.9655	1.2958	1.6546	2.2912	1.5789	1.2999
	5	1.8045	1.7509	2.0923	1.3984	1.6997	2.4150	1.7089	1.4163
EA(v)	1	-0.1224	-0.1244	0.2280	-0.1303	-0.1772	0.6110	-0.0876	-0.2824
	2	0.8815	0.8505	1.2043	0.6242	0.7978	1.5658	0.8531	0.6002
	3	1.3163	1.2615	1.6192	0.9460	1.2118	1.9601	1.2568	0.9742
	4	1.5566	1.5046	1.8457	1.1266	1.4542	2.1825	1.4794	1.1818
	5	1.7103	1.6567	1.9963	1.2641	1.6003	2.3247	1.6227	1.3145