Table S1. The bond length/Å of neutral and ionized optimized geometries for studied molecules 1-1 to 1-6

	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
1-1	1.422	1.362	1.438	1.405	1.429	1.429	1.405	1.438	1.362				1.444	1.474	1.444	1.422
1-1h	1.407	1.376	1.422	1.424	1.425	1.425	1.424	1.422	1.376				1.437	1.471	1.437	1.407
1-1e	1.405	1.379	1.425	1.426	1.426	1.426	1.426	1.425	1.379				1.442	1.475	1.442	1.405
1-2	1.433	1.366	1.436	1.39	1.417	1.416	1.416	1.417	1.39	1.436	1.366	1.433	1.453	1.458	1.458	1.453
1-2h	1.42	1.377	1.423	1.404	1.406	1.422	1.422	1.406	1.404	1.423	1.377	1.42	1.446	1.456	1.456	1.446
1-2e	1.419	1.38	1.425	1.406	1.41	1.423	1.423	1.41	1.406	1.425	1.38	1.419	1.448	1.464	1.464	1.448
1-3	1.433	1.366	1.436	1.388	1.418	1.414	1.414	1.418	1.388	1.436	1.366	1.433	1.451	1.459	1.459	1.451
1-3h	1.42	1.377	1.423	1.403	1.407	1.42	1.42	1.407	1.403	1.423	1.377	1.42	1.443	1.457	1.457	1.443
1-3e	1.419	1.379	1.425	1.405	1.41	1.421	1.421	1.41	1.405	1.425	1.379	1.419	1.445	1.464	1.464	1.445
1-4	1.429	1.365	1.436	1.4	1.427	1.404	1.404	1.427	1.4	1.436	1.365	1.429	1.457	1.455	1.455	1.457
1-4h	1.415	1.376	1.426	1.42	1.42	1.408	1.408	1.42	1.42	1.426	1.376	1.415	1.449	1.453	1.453	1.449
1-4e	1.414	1.378	1.429	1.419	1.421	1.41	1.41	1.421	1.419	1.429	1.378	1.414	1.45	1.46	1.46	1.45
1-5	1.423	1.373	1.452	1.39	1.417	1.414	1.414	1.417	1.39	1.452	1.373	1.423	1.459	1.454	1.454	1.459
1-5h	1.409	1.386	1.439	1.403	1.408	1.419	1.419	1.408	1.403	1.439	1.396	1.409	1.452	1.453	1.453	1.452
1-5e	1.407	1.388	1.442	1.405	1.41	1.42	1.42	1.41	1.405	1.442	1.388	1.407	1.455	1.457	1.457	1.455
1-6	1.457	1.381	1.449	1.391	1.417	1.414	1.414	1.417	1.391	1.449	1.381	1.457	1.45	1.454	1.454	1.45
1-6h	1.444	1.395	1.436	1.405	1.407	1.419	1.419	1.407	1.405	1.436	1.395	1.444	1.444	1.453	1.453	1.444
1-6e	1.439	1.396	1.437	1.406	1.41	1.419	1.419	1.41	1.406	1.437	1.396	1.439	1.447	1.458	1.458	1.447

Table S2. The bond angle/ °of neutral and ionized optimized geometries for studied molecules 1-1 to 1-6

	17	18	19	20	21
1-1	121.8	120.5	120.5	121.8	
1-1h	121.4	120	120	121.4	
1-1e	122.4	121.2	121.2	122.4	
1-2	121	122.3	120.4	122.3	121
1-2h	120.5	122.1	119.8	122.1	120.5
1-2e	121.6	122.9	121.7	122.9	121.6
1-3	120.9	122.4	120.2	122.4	120.9
1-3h	120.4	122.3	119.5	122.3	120.4
1-3e	121.5	123.1	121.5	123.1	121.5
1-4	121.6	120.1	122.9	120.1	121.6
1-4h	121.3	119.3	123.3	119.3	121.3
1-4e	122.1	120.9	123.9	120.9	122.1
1-5	118.6	123.1	119.9	123.1	118.6
1-5h	117.9	123	119.4	123	117.9
1-5e	119.2	123.8	121	123.8	119.2
1-6	120.1	122.9	119.9	122.9	120.1
1-6h	119.5	122.9	119.5	122.9	119.5
1-6e	120.7	123.5	120.9	123.5	120.7

Table S3. The energies of IP, EA, HOMO, LUMO, H-L, and reorganization energies (λ_+ and λ_-) of the studied molecules 1-1 to 1-6 (all in eV)

Compounds	IP	EA	HOMO	LUMO	H-L	λ_+	λ_-
1-1	6.03	1.28	-4.942	-2.34	2.60	0.156	0.203
1-2	5.76	1.16	-4.565	-2.355	2.21	0.100	0.138
1-3	5.65	1.19	-4.496	-2.325	2.17	0.105	0.142
1-4	5.47	1.23	-4.425	-2.271	2.15	0.150	0.161
1-5	5.42	1.34	-4.424	-2.3	2.12	0.093	0.165
1-6	5.26	1.41	-4.387	-2.272	2.115	0.115	0.145

Table S4. The largest calculated electron and hole mobility (in $cm^2 V^{-1} s^{-1}$) for the anisotropic mobility in ab plane μ^a and all three planes μ^b of molecule 1-4.

	μ^a_{ele}	μ^b_{ele}	μ^a_{hole}	μ^b_{hole}
1	0.90	0.90	6.57	6.57
2	4.40	4.40	1.89	1.88
3	0.098	0.097	0.045	0.044
4	2.624E-4	1.070E-4	0.076	0.051

Table S5. The energies (all in eV) of IPs, EAs, HOMOs, LUMOs, H-Ls, and Reorganization Energies (λ_+ and λ_-) of the Studied Molecules

Compounds	IP	EA	HOMO	LUMO	H-L	λ_+	λ_-
1	6.03	1.28	-4.94	-2.34	2.60	0.156	0.203
2	6.13	1.42	-4.86	-2.66	2.20	0.098	0.137
3	7.92	3.27	-6.96	-4.27	2.69	0.243	0.327
4	5.98	1.50	-4.88	-2.46	2.43	0.202	0.587

Table S6. The structural parameters(θ_i/°, γ_i/°and r_i/Å) and corresponding transfer integrals (V_h/meV and V_e/meV) for molecules 1-4 along different hopping pathways

	pathway	θ_i	γ_i	r_i	V_h	V_e
1	P	0	0	7.174	86.62	42.78
	T1	63.435	0	8.054	16.39	6.68
	T2	116.565	0	8.054	16.39	6.68
	L1	0	75.024	13.88	1.42	0.58
	L2	0	104.976	13.88	1.42	0.58
	R1	63.435	65.043	15.207	0.30	0.25
	R2	63.435	65.043	15.207	0.30	0.25
2	P	0	0	6.265	34.15	46.09
	T1	47.931	0	5.221	77.47	77.67
	T2	125.522	0	4.762	45.53	75.43
	L1	0	66.733	16.109	1.30	8.57
	L2	0	89.619	14.799	3.30	0.62
	L3	0	112.621	16.032	0.01	0
3	P	0	0	7.070	5.79	6.15
	T1	75.359	0	13.987	0.99	1.22
	T2	104.641	0	13.987	0.121	1.69
	L1	75.359	59.680	15.068	0	0
	L2	90	59.680	13.306	0.49	0.76
4	P	0	0	7.880	11.67	0.36
	T1	55.440	0	6.946	3.18	7.46

T2	124.560	0	6.946	3.18	7.46
L1	0	66.485	9.875	26.10	10.77
L2	0	113.515	9.875	26.10	10.80

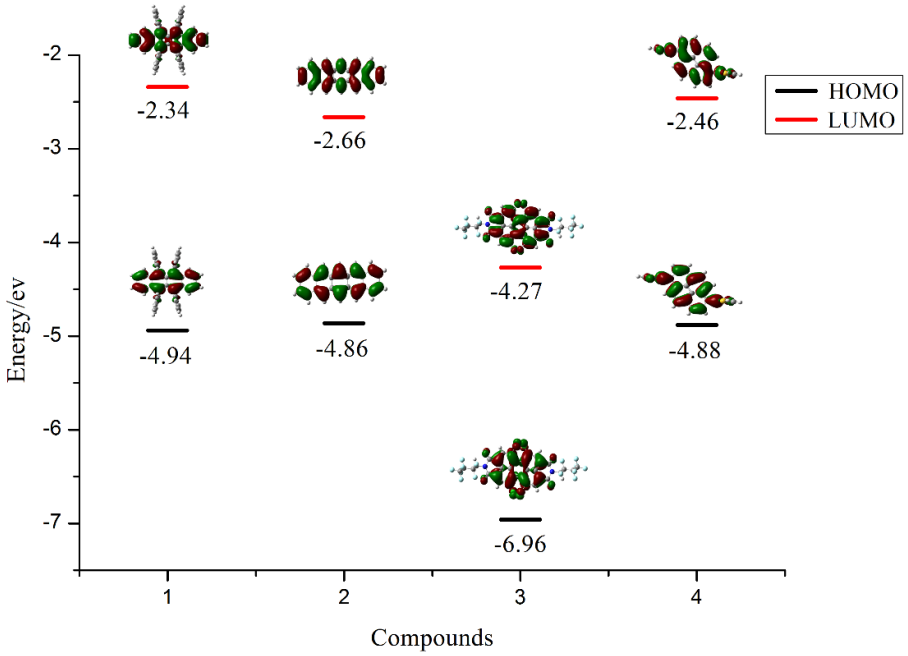

Figure S1. The energies (all in eV) and their electronic density contours of HOMOs and LUMOs for studied molecules1-4