Supplementary Information of On the Characteristic and Dynamics of Excited States Populated After Excitation at Soret Band of Bis-Dicarbacorrole Cu(III) and Pd(II) Metal Complexes

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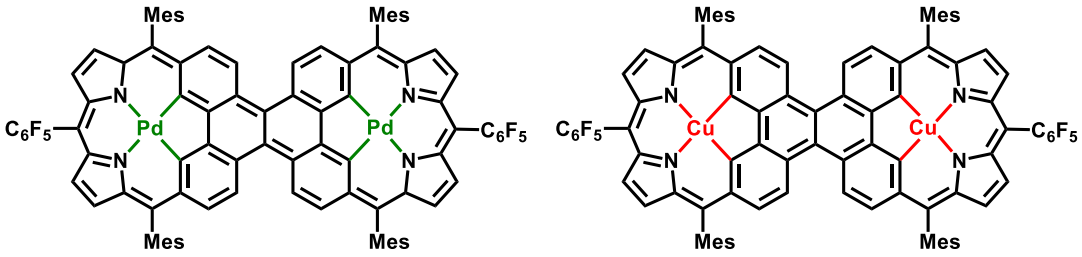


Fig.S1: Structure of **Bis-Pd** and **Bis-Cu** reported in previous research.

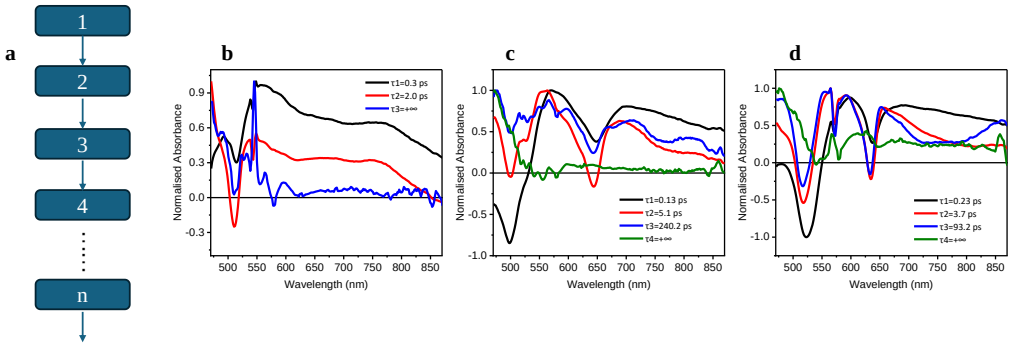


Fig.S2: a). An example of sequential model (left) and normalized EAS of b). **Mono-Cu**, c). **Mono-Pd**, and d). **Mix-Cu-Pd** in DCM extracted from corresponding TA spectra.

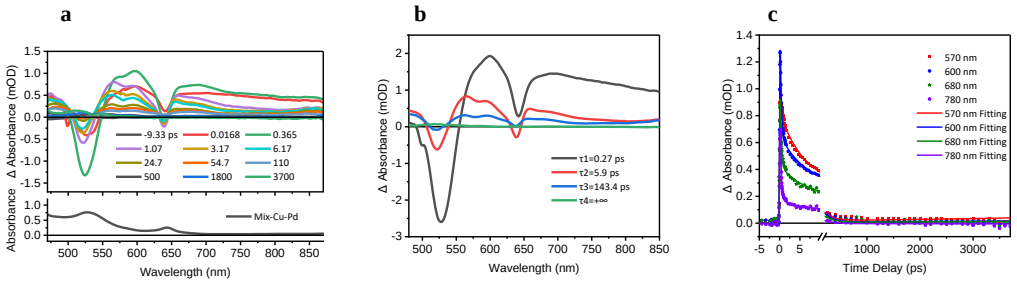


Fig.S3: a). TA spectra of **Mix-Cu-Pd** in toluene with excitation at 435 nm, b). EAS of TA of **Mix-Cu-Pd** in toluene, c). Kinetic trace (scattered dots) and fitting trace (solid line) of **Mix-Cu-Pd** in toluene TA at selected wavelength.

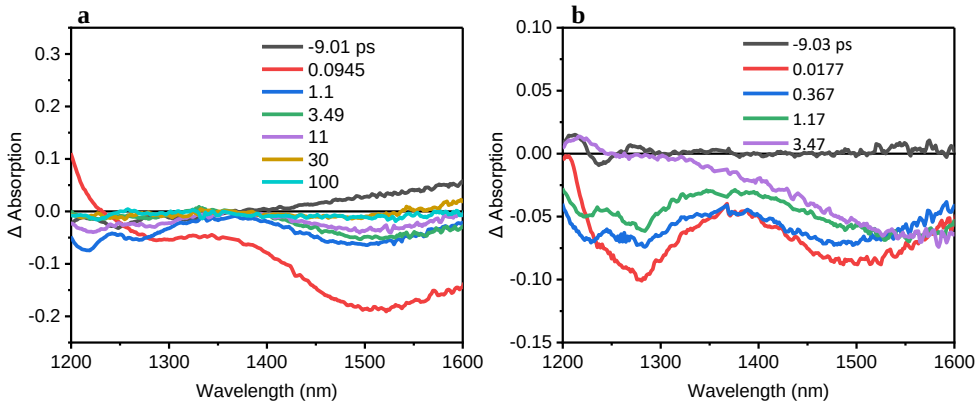


Fig.S4: Femtosecond transient absorption spectra of a). **Mix-Cu-Pd** and b). **Mono-Pd** in DCM with excitation at 435 nm and probe in NIR range (1200-1600 nm).

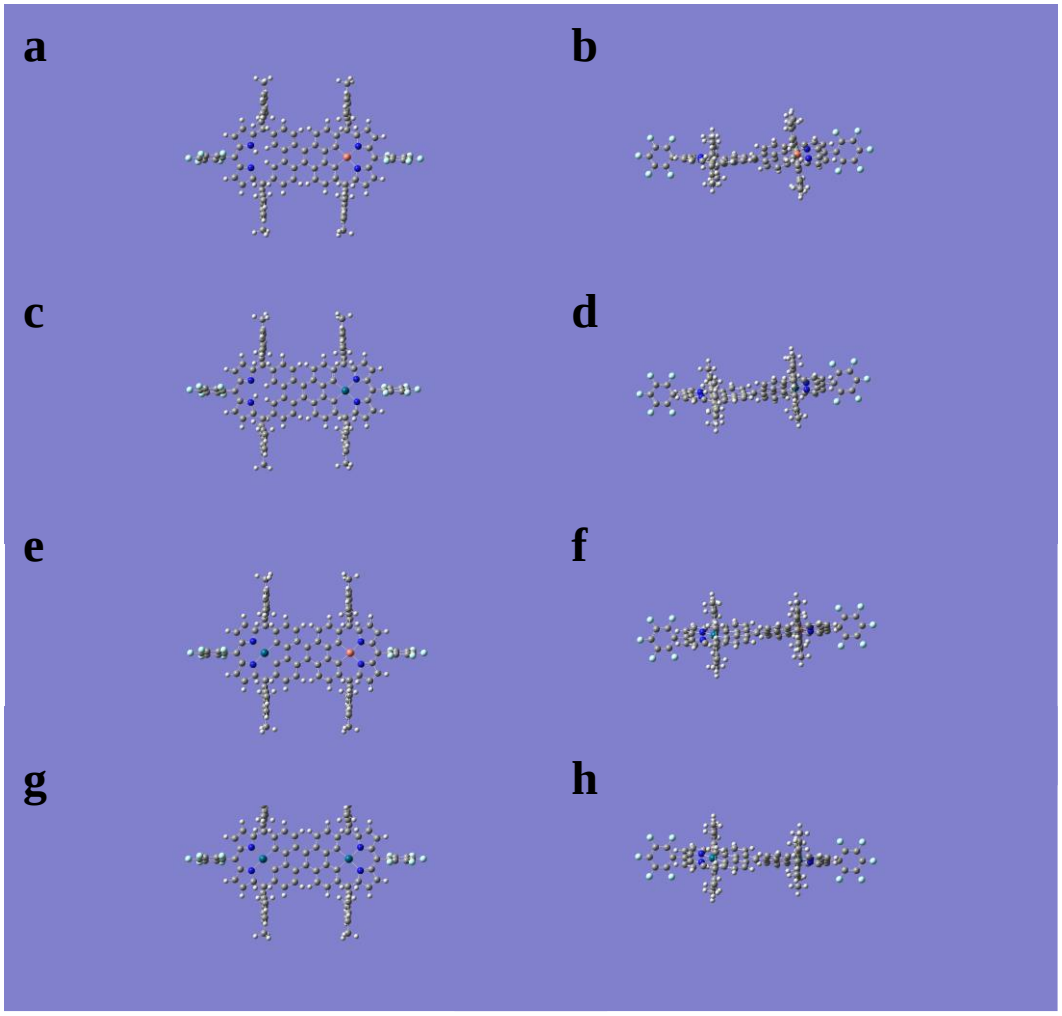


Fig.S5: Optimized ground state structure of **Bis-H$_3$** metal complexes in DCM by using DFT calculation and here for a,b). **Mono-Cu**, c,d). **Mono-Pd**, e,f). **Mix-Cu-Pd**, and g,h). **Bis-Pd**

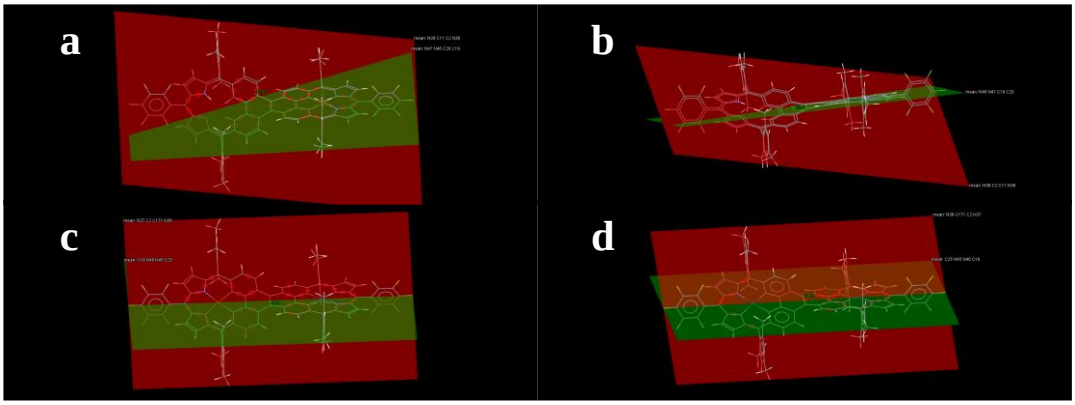


Fig.S6: Dihedral angle between the two corrole subunits of the DFT calculation optimized **Bis-H_3** metal complexes structure of a). **Mono-Cu** (31.93°), b). **Mono-Pd** (32.30°), c). **Mix-Cu-Pd** (28.34°), and d). **Bis-Pd** (29.32°). The value in the bracket after the name of the compound is the value of the dihedral angle between the two corrole subunits in that compound.

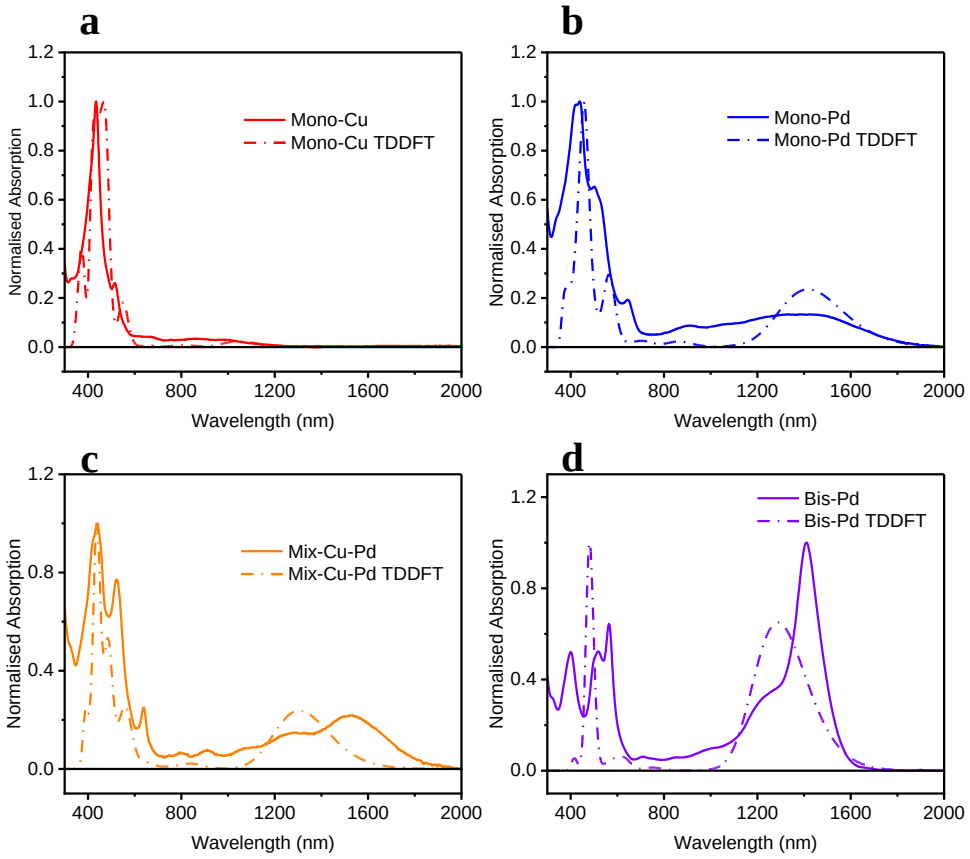


Fig.S7: Experimental UV-Vis-NIR absorption spectra (solid line) and simulated UV-Vis-NIR absorption spectra (dashed line) of a). **Mono-Cu**, b). **Mono-Pd**, c). **Mix-Cu-Pd**, and d). **Bis-Pd** in DCM suggested by TD-DFT calculation.

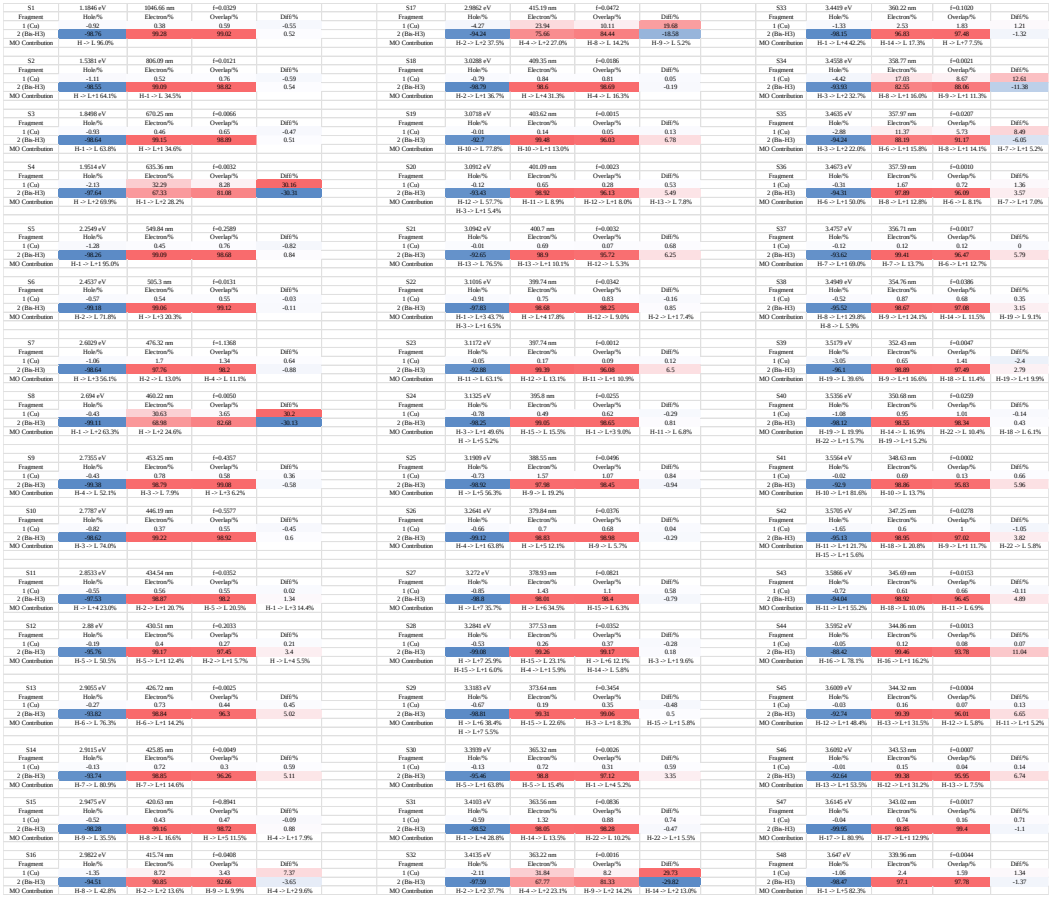


Fig.S8: Fragment analysis of 48 excited states' electron-hole distribution of **Mono-Cu** in DCM based on TD-DFT calculation, here positive value indicates gain of electron density and negative value indicates loss of electron density. And in molecular orbital (MO) contribution, H indicates HOMO and L indicates LUMO.

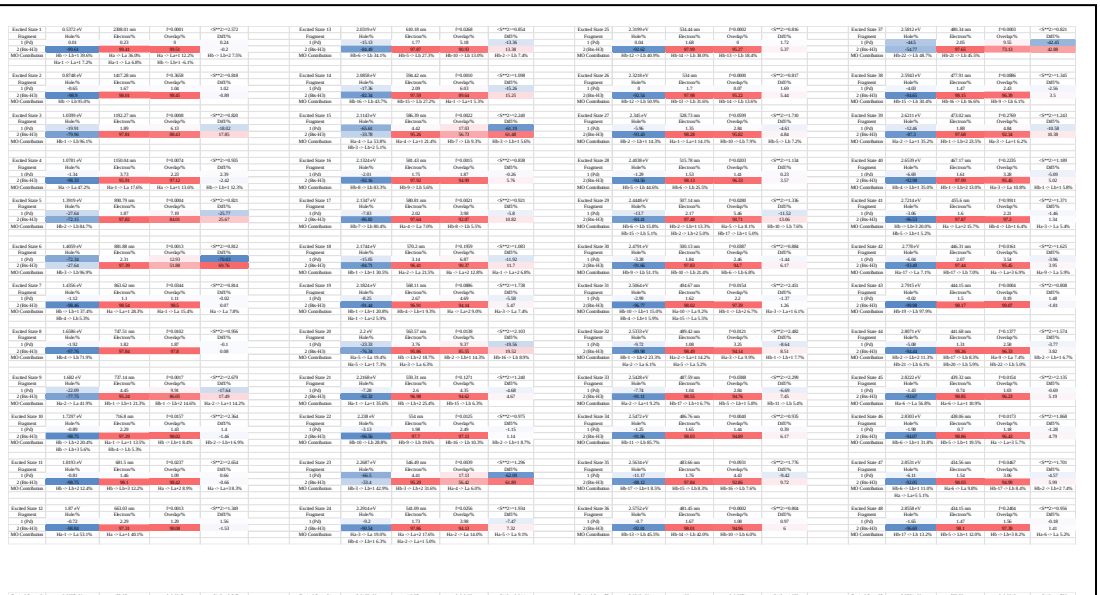


Fig.S9: Fragment analysis of 96 excited states' electron-hole distribution of **Mono-Pd** in DCM based on TD-DFT calculation, here positive value indicates gain of electron density and negative value indicates loss of electron density. And in molecular orbital (MO) contribution, H indicates HOMO and L indicates LUMO.

S1	0.9631 eV	1287.33 nm	f=1.3987	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-0.74	0.86	0.8	0.12
2 (Pd)	-0.74	0.86	0.8	0.12
3 (Bis-H3)	-95.65	95.63	95.64	-0.02
MO Contribution	H -> L 104.9%	H <- L -7.2%		

S2	1.1074 eV	1119.61 nm	f=0.0000	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-10.18	0.84	2.92	-9.34
2 (Pd)	-10.22	0.84	2.92	-9.38
3 (Bis-H3)	-75.98	95.65	85.25	19.66
MO Contribution	H-1 -> L 98.7%			

S3	1.178 eV	1052.46 nm	f=0.0080	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-11.2	0.88	3.13	-10.32
2 (Pd)	-11.15	0.88	3.13	-10.27
3 (Bis-H3)	-74.16	95.58	84.19	21.42
MO Contribution	H-2 -> L 98.4%			

S4	1.3529 eV	916.43 nm	f=0.0019	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-0.77	2.34	1.34	1.57
2 (Pd)	-0.77	2.34	1.34	1.57
3 (Bis-H3)	-95.66	91.69	93.65	-3.97
MO Contribution	H -> L+1 91.1%	H-4 -> L 8.2%		

S5	1.4926 eV	830.67 nm	f=0.0004	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-35.53	0.8	5.35	-34.73
2 (Pd)	-35.12	0.8	5.32	-34.32
3 (Bis-H3)	-23.73	95.61	47.63	71.87
MO Contribution	H-5 -> L 98.9%			

S6	1.5318 eV	809.42 nm	f=0.0009	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-37.13	0.8	5.46	-36.33
2 (Pd)	-37.54	0.8	5.49	-36.74
3 (Bis-H3)	-20.2	95.62	43.95	75.42
MO Contribution	H-6 -> L 98.6%			

S7	1.5402 eV	804.99 nm	f=0.0000	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-14.23	0.92	3.61	-13.31
2 (Pd)	-14.21	0.92	3.61	-13.29
3 (Bis-H3)	-71.19	95.37	82.4	24.18
MO Contribution	H-3 -> L 95.9%			

S8	1.6449 eV	753.74 nm	f=0.0090	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-2.69	0.98	1.62	-1.71
2 (Pd)	-2.69	0.98	1.62	-1.72
3 (Bis-H3)	-93.94	95.13	94.53	1.19
MO Contribution	H-4 -> L 88.4%	H -> L+1 7.6%		

S9	1.6588 eV	747.44 nm	f=0.0204	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-21.41	0.89	4.37	-20.52
2 (Pd)	-21.42	0.89	4.37	-20.53
3 (Bis-H3)	-56.49	95.51	73.45	39.02
MO Contribution	H-7 -> L 99.0%			

S10	1.97 eV	629.35 nm	f=0.1052	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-0.82	1.95	1.26	1.14
2 (Pd)	-0.83	1.95	1.27	1.12
3 (Bis-H3)	-98.45	93.07	94.35	-2.58
MO Contribution	H -> L+2 82.7%	H-16 -> L 11.0%		

S11	2.0235 eV	612.72 nm	f=0.0000	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-0.1	0.77	0.27	0.67
2 (Pd)	-0.04	0.77	0.17	0.73
3 (Bis-H3)	-93.66	95.92	94.78	2.27
MO Contribution	H-8 -> L 98.6%			

S12	2.0249 eV	612.31 nm	f=0.0002	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-0.03	0.77	0.16	0.74
2 (Pd)	-0.09	0.77	0.27	0.67
3 (Bis-H3)	-93.66	95.94	94.79	2.28
MO Contribution	H-9 -> L 98.8%			

S13	2.0255 eV	612.13 nm	f=0.0026	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-1.13	0.78	0.94	-0.34
2 (Pd)	-0.34	0.78	0.52	0.44
3 (Bis-H3)	-92.44	95.84	94.12	3.4
MO Contribution	H-11 -> L 77.3%	H-10 -> L 20.2%		

S14	2.0265 eV	611.8 nm	f=0.0167	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-0.31	0.82	0.51	0.5
2 (Pd)	-1.11	0.81	0.95	-0.29
3 (Bis-H3)	-92.56	95.75	94.14	3.19
MO Contribution	H-10 -> L 74.5%	H-11 -> L 20.8%		

S15	2.1455 eV	577.87 nm	f=0.0329	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-4.71	1.07	2.25	-3.64
2 (Pd)	-4.7	1.07	2.25	-3.63
3 (Bis-H3)	-90.59	95.45	91.92	6.14
MO Contribution	H-16 -> L 66.7%	H-3 -> L+1 9.0%	H-12 -> L 6.7%	H -> L+2 6.5%
	H-13 -> L 5.6%			

S16	2.157 eV	574.79 nm	f=0.0000	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-21.16	2.34	7.04	-18.81
2 (Pd)	-21.06	2.34	7.03	-18.72
3 (Bis-H3)	-53.57	91.72	70.09	38.15
MO Contribution	H-2 -> L+1 49.6%	H-5 -> L+1 28.3%	H-17 -> L 10.1%	H-6 -> L+2 7.6%

S17	2.1653 eV	572.59 nm	f=0.0001	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-0.07	0.77	0.23	0.7
2 (Pd)	-0.07	0.77	0.23	0.7
3 (Bis-H3)	-97.49	95.94	94.2	3.46
MO Contribution	H-12 -> L 51.1%	H-13 -> L 48.1%		

S18	2.1672 eV	572.11 nm	f=0.0000	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-0.06	0.77	0.21	0.71
2 (Pd)	0.01	0.78	0	0.79
3 (Bis-H3)	-92.54	95.87	94.19	3.34
MO Contribution	H-14 -> L 82.4%	H-15 -> L 15.3%		

S19	2.1675 eV	572.01 nm	f=0.0004	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	0.01	0.78	0	0.78
2 (Pd)	-0.06	0.77	0.22	0.71
3 (Bis-H3)	-92.55	95.99	94.25	3.44
MO Contribution	H-15 -> L 72.1%	H-14 -> L 16.9%	H-13 -> L 5.6%	

S20	2.1681 eV	571.86 nm	f=0.0051	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-0.33	0.83	0.52	0.5
2 (Pd)	-0.32	0.83	0.52	0.5
3 (Bis-H3)	-92.3	95.68	93.97	3.38
MO Contribution	H-13 -> L 39.8%	H-12 -> L 36.3%	H-15 -> L 12.0%	H-16 -> L 8.7%

S21	2.1816 eV	568.31 nm	f=0.0568	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-12.36	2.44	5.49	-9.92
2 (Pd)	-12.42	2.44	5.51	-9.98
3 (Bis-H3)	-71.3	91.5	80.89	20
MO Contribution	H-1 -> L+1 85.0%	H-6 -> L+1 6.3%		

S22	2.2025 eV	562.93 nm	f=0.0000	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-26.11	2.28	7.72	-23.82
2 (Pd)	-25.64	2.26	7.61	-23.38
3 (Bis-H3)	-44.38	91.88	63.85	47.5
MO Contribution	H-5 -> L+1 48.3%	H-2 -> L+1 19.5%	H-17 -> L 16.4%	H-6 -> L+2 11.7%

S23	2.2113 eV	560.67 nm	f=0.0081	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-35.53	2.59	9.59	-32.95
2 (Pd)	-36.07	2.62	9.71	-33.46
3 (Bis-H3)	-23.52	90.81	46.21	67.3
MO Contribution	H-6 -> L+1 69.1%	H-5 -> L+2 20.9%	H-1 -> L+1 8.0%	

S24	2.3256 eV	533.14 nm	f=0.0086	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-12.81	1.7	4.67	-11.11
2 (Pd)	-12.77	1.7	4.66	-11.07
3 (Bis-H3)	-72.91	93.38	82.51	20.47
MO Contribution	H-3 -> L+1 45.2%	H-19 -> L 43.4%	H-7 -> L+2 6.0%	

S25	2.3394 eV	529.98 nm	f=0.0000	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-11.49	1.28	3.84	-10.2
2 (Pd)	-11.47	1.28	3.84	-10.19
3 (Bis-H3)	-75.7	94.5	84.58	18.8
MO Contribution	H-17 -> L 62.2%	H-2 -> L+1 21.8%	H -> L+3 6.6%	

S26	2.3524 eV	527.06 nm	f=0.0014	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-8.87	0.97	2.94	-7.9
2 (Pd)	-8.92	0.97	2.94	-7.95
3 (Bis-H3)	-79.23	95.43	86.97	16.16
MO Contribution	H-18 -> L 88.4%	H-7 -> L+1 7.0%		

S27	2.455 eV	505.02 nm	f=0.0077	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-20.45	2.31	6.88	-18.14
2 (Pd)	-20.45	2.31	6.88	-18.14
3 (Bis-H3)	-58.39	91.83	73.23	33.44
MO Contribution	H-7 -> L+1 71.5%	H-3 -> L+2 11.0%	H-18 -> L 8.5%	

S28	2.5301 eV	490.03 nm	f=0.4575	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-8.59	1.45	3.53	-7.14
2 (Pd)	-8.61	1.45	3.53	-7.16
3 (Bis-H3)	-81.31	94.17	87.5	12.86
MO Contribution	H-19 -> L 48.8%	H-3 -> L+1 24.8%	H-16 -> L 8.0%	H-17 -> L+1 5.2%

S29	2.587 eV	479.26 nm	f=1.7696	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-2.23	2.45	2.34	0.22
2 (Pd)	-2.22	2.45	2.34	0.23
3 (Bis-H3)	-94.82	91.35	93.07	-3.47
MO Contribution	H-4 -> L+1 86.3%	H-2 -> L+2 8.6%		

S30	2.6835 eV	462.02 nm	f=0.0031	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-20.58	0.85	4.18	-19.73
2 (Pd)	-20.3	0.85	4.15	-19.45
3 (Bis-H3)	-54.04	95.57	71.87	41.54
MO Contribution	H-24 -> L 95.9%			

S31	2.6934 eV	460.33 nm	f=0.0000	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-8.69	1.97	4.14	-6.71
2 (Pd)	-8.72	1.97	4.15	-6.74
3 (Bis-H3)	-78.73	93.15	85.67	14.37
MO Contribution	H-1 -> L+2 78.3%	H -> L+3 11.8%	H-2 -> L+1 7.0%	

S32	2.6944 eV	460.15 nm	f=0.0000	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-23.07	0.85	4.42	-22.22
2 (Pd)	-23.44	0.85	4.46	-22.59
3 (Bis-H3)	-49.15	95.59	68.55	46.44
MO Contribution	H-25 -> L 91.8%	H-20 -> L 6.8%		

S33	2.698 eV	459.54 nm	f=0.0000	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-1.6	1.03	1.29	-0.57
2 (Pd)	-1.61	1.03	1.29	-0.58
3 (Bis-H3)	-94.42	96.21	95.31	1.79
MO Contribution	H -> L+3 66.2%	H-1 -> L+2 13.2%	H-4 -> L+2 10.7%	

S34	2.7173 eV	456.28 nm	f=0.0014	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-1.94	0.7	1.16	-1.24
2 (Pd)	-0.36	0.75	0.52	0.39
3 (Bis-H3)	-97.55	96.04	96.79	-1.51
MO Contribution	H-20 -> L 78.2%	H-21 -> L 15.4%		

S35	2.7181 eV	456.15 nm	f=0.0019	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-0.07	0.75	0.23	0.68
2 (Pd)	-1.58	0.7	1.05	-0.89
3 (Bis-H3)	-86.7	96.3	91.37	9.6
MO Contribution	H-21 -> L 80.9%	H-20 -> L 14.1%		

S36	2.7595 eV	449.29 nm	f=0.0035	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-9.08	2.18	4.45	-6.9
2 (Pd)	-9.05	2.18	4.44	-6.87
3 (Bis-H3)	-78.24	92.46	85.05	14.22
MO Contribution	H-2 -> L+2 83.4%	H-4 -> L+1 8.8%		

S37	2.8876 eV	429.36 nm	f=0.0018	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-1	3.03	1.74	2.03
2 (Pd)	-0.32	1.81	0.76	1.49
3 (Bis-H3)	-93.41	92.35	92.48	-0.26
MO Contribution	H-11 -> L+1 72.4%	H-10 -> L+2 10.7%	H-10 -> L+1 9.1%	

S38	2.8891 eV	429.15 nm	f=0.0001	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-0.38	1.86	0.84	1.48
2 (Pd)	-1.06	3.08	1.81	2.02
3 (Bis-H3)	-92.48	90.68	91.57	-1.8
MO Contribution	H-10 -> L+1 74.5%	H-11 -> L+2 11.3%	H-11 -> L+1 9.0%	

S39	2.8905 eV	428.94 nm	f=0.0008	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-0.12	3.23	0.63	3.11
2 (Pd)	-0.05	1.71	0.28	1.66
3 (Bis-H3)	-93.69	92.41	93.05	-1.28
MO Contribution	H-8 -> L+1 86.2%	H-9 -> L+2 8.1%		

S40	2.8916 eV	428.77 nm	f=0.0001	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-0.05	1.71	0.28	1.66
2 (Pd)	-0.12	3.23	0.63	3.11
3 (Bis-H3)	-93.65	90.45	92.04	-3.19
MO Contribution	H-9 -> L+1 86.0%	H-8 -> L+2 8.2%		

S41	2.9067 eV	426.54 nm	f=0.0137	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-1.28	0.8	1.01	-0.48
2 (Pd)	-1.29	0.8	1.02	-0.48
3 (Bis-H3)	-92.98	95.94	93.99	3.86
MO Contribution	H-22 -> L 91.4%			

S42	2.9498 eV	420.31 nm	f=0.0001	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-34.08	0.92	5.6	-33.16
2 (Pd)	-33.93	0.92	5.58	-33.01
3 (Bis-H3)	-29.53	95.31	53.05	65.78
MO Contribution	H-27 -> L 98.3%			

S43	2.9542 eV	419.68 nm	f=0.0000	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-0.88	0.81	0.84	-0.07
2 (Pd)	-0.9	0.81	0.85	-0.09
3 (Bis-H3)	-92.82	95.96	94.37	3.14
MO Contribution	H-23 -> L 86.7%			

S44	2.9893 eV	414.76 nm	f=0.1053	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-12.88	2.4	5.56	-10.48
2 (Pd)	-12.88	2.4	5.56	-10.48
3 (Bis-H3)	-73.67	91.6	82.14	17.93
MO Contribution	H-17 -> L+1 41.0%	H-7 -> L+2 37.6%	H-3 -> L+1 15.2%	

S45	3.0151 eV	411.22 nm	f=0.0000	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-8.03	0.9	2.69	-7.13
2 (Pd)	-8.03	0.9	2.69	-7.13
3 (Bis-H3)	-76.9	95.45	85.67	18.55
MO Contribution	H-28 -> L 83.9%	H-23 -> L 6.2%		

S46	3.0429 eV	407.46 nm	f=0.0039	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-10.51	2.16	4.77	-8.35
2 (Pd)	-10.51	2.16	4.77	-8.34
3 (Bis-H3)	-75.35	92.44	85.1	14.09
MO Contribution	H-3 -> L+2 78.0%	H-7 -> L+1 15.8%		

S47	3.0531 eV	406.09 nm	f=0.0000	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-2.32	2.48	2.4	0.15
2 (Pd)	-2.31	2.36	2.33	0.05
3 (Bis-H3)	-91.57	91.66	90.63	2.09
MO Contribution	H-12 -> L+1 38.4%	H-13 -> L+1 29.9%	H-16 -> L+1 8.9%	H-19 -> L+1 5.2%

S48	3.058 eV	405.44 nm	f=0.0013	
Fragment	Hole%	Electron%	Overlap%	Diff%
1 (Pd)	-0.18	2.43	0.66	2.25
2 (Pd)	-0.2	2.53	0.72	2.33
3 (Bis-H3)	-92.36	91.33	91.85	-1.03
MO Contribution	H-13 -> L+1 48.7%	H-12 -> L+1 39.5%		

Fig.S10: Fragment analysis of 48 excited states' electron-hole distribution of **Bis-Pd** in DCM based on TD-DFT calculation, here positive value indicates gain of electron density and negative value indicates loss of electron density. And in molecular orbital (MO) contribution, H indicates HOMO and L indicates LUMO.

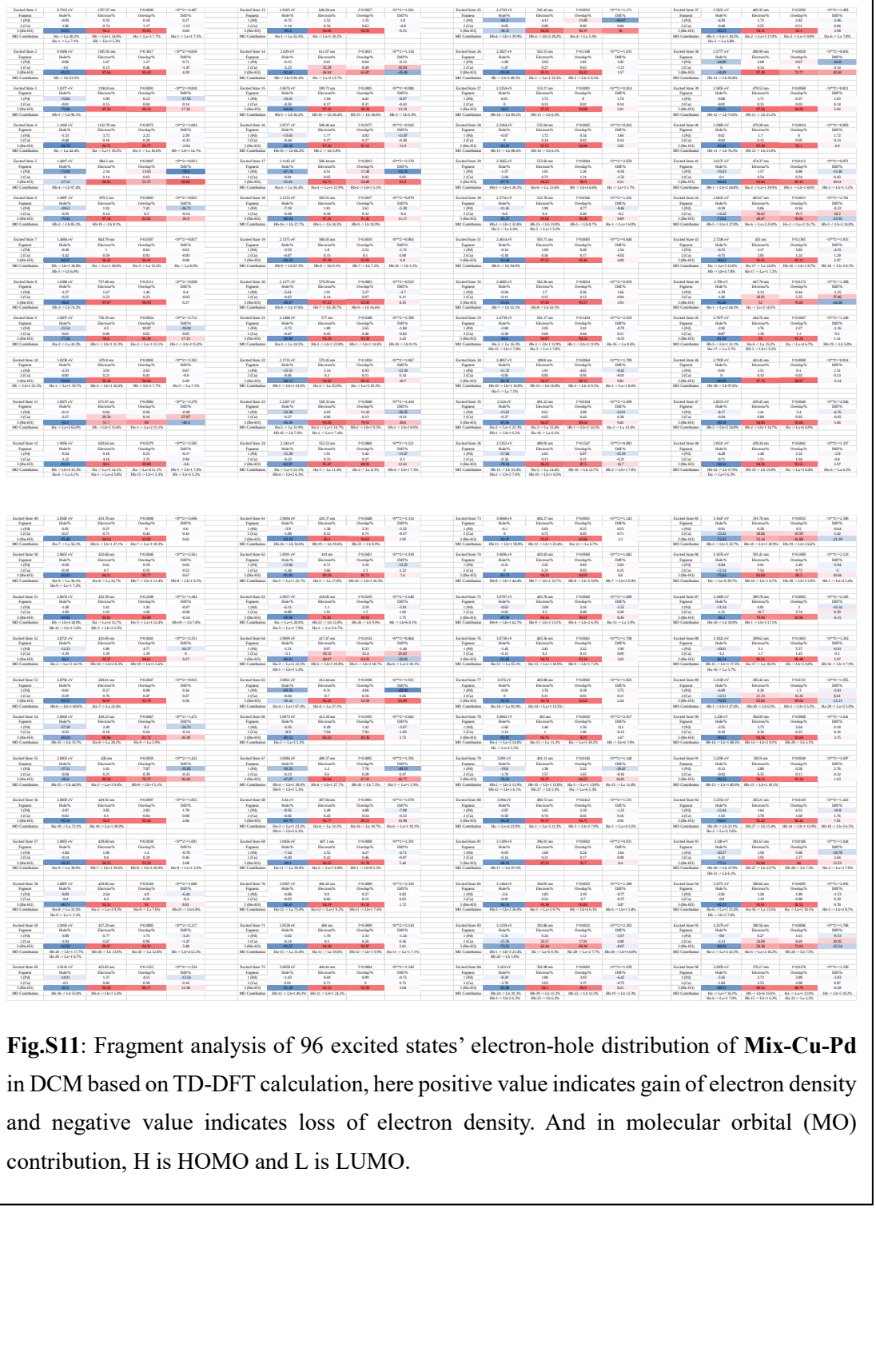


Fig.S11: Fragment analysis of 96 excited states' electron-hole distribution of **Mix-Cu-Pd** in DCM based on TD-DFT calculation, here positive value indicates gain of electron density and negative value indicates loss of electron density. And in molecular orbital (MO) contribution, H is HOMO and L is LUMO.

D1	0.8748 eV	1417.28 nm	f=0.3658	<S**2>=0.818
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-0.65	1.67	1.04	1.02
2 (Bis-H3)	-98.9	98.01	98.45	-0.89

D2	1.0399 eV	1192.27 nm	f=0.0008	<S**2>=0.820
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-19.91	1.89	6.13	-18.02
2 (Bis-H3)	-79.96	97.81	88.43	17.85

D3	1.0781 eV	1150.04 nm	f=0.0074	<S**2>=0.935
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-1.34	3.73	2.23	2.39
2 (Bis-H3)	-98.33	95.91	97.12	-2.42

D4	1.3919 eV	890.79 nm	f=0.0004	<S**2>=0.821
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-27.64	1.87	7.19	-25.77
2 (Bis-H3)	-72.15	97.82	84.01	25.67

D5	1.4059 eV	881.88 nm	f=0.0013	<S**2>=0.812
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-72.34	2.31	12.93	-70.03
2 (Bis-H3)	-27.64	97.39	51.88	69.76

D6	1.4356 eV	863.62 nm	f=0.0344	<S**2>=0.814
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-1.12	1.1	1.11	-0.02
2 (Bis-H3)	-98.46	98.54	98.5	0.07

D7	1.6586 eV	747.51 nm	f=0.0102	<S**2>=0.956
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-1.92	1.82	1.87	-0.1
2 (Bis-H3)	-97.76	97.84	97.8	0.08

D8	1.87 eV	663.03 nm	f=0.0013	<S**2>=1.349
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-0.72	2.29	1.29	1.56
2 (Bis-H3)	-98.84	97.31	98.08	-1.53

D9	2.0319 eV	610.18 nm	f=0.0268	<S**2>=0.854
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-15.13	1.77	5.18	-13.36
2 (Bis-H3)	-84.49	97.87	90.93	13.38

D10	2.0858 eV	594.42 nm	f=0.0010	<S**2>=1.098
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-17.36	2.09	6.03	-15.26
2 (Bis-H3)	-82.34	97.59	89.64	15.25

D11	2.1324 eV	581.43 nm	f=0.0015	<S**2>=0.838
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-2.01	1.75	1.87	-0.26
2 (Bis-H3)	-92.16	97.92	94.99	5.76

D12	2.1347 eV	580.81 nm	f=0.0021	<S**2>=0.921
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-7.83	2.02	3.98	-5.8
2 (Bis-H3)	-86.82	97.64	92.07	10.82

D13	2.1744 eV	570.2 nm	f=0.1959	<S**2>=1.083
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-15.05	3.14	6.87	-11.92
2 (Bis-H3)	-84.71	96.41	90.37	11.7

D14	2.2168 eV	559.31 nm	f=0.1271	<S**2>=1.240
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-7.28	2.6	4.35	-4.68
2 (Bis-H3)	-92.32	96.98	94.62	4.67

D15	2.238 eV	554 nm	f=0.0125	<S**2>=0.975
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-3.13	1.98	2.49	-1.15
2 (Bis-H3)	-96.56	97.7	97.13	1.14

D16	2.2687 eV	546.49 nm	f=0.0039	<S**2>=1.296
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-66.5	4.41	17.13	-62.09
2 (Bis-H3)	-33.4	95.29	56.42	61.89

D17	2.3199 eV	534.44 nm	f=0.0002	<S**2>=0.816
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	0.04	1.68	0	1.72
2 (Bis-H3)	-92.62	97.99	95.27	5.37

D18	2.3218 eV	534 nm	f=0.0000	<S**2>=0.817
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	0	1.7	0.07	1.69
2 (Bis-H3)	-92.54	97.98	95.22	5.44

D19	2.4038 eV	515.78 nm	f=0.0203	<S**2>=1.134
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-1.29	1.53	1.41	0.23
2 (Bis-H3)	-94.56	98.13	96.33	3.57

D20	2.4448 eV	507.14 nm	f=0.0280	<S**2>=1.336
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-13.7	2.17	5.46	-11.52
2 (Bis-H3)	-84.41	97.48	90.71	13.06

D21	2.4791 eV	500.13 nm	f=0.0387	<S**2>=0.884
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-3.28	1.84	2.46	-1.44
2 (Bis-H3)	-91.66	97.83	94.7	6.17

D22	2.5472 eV	486.76 nm	f=0.0040	<S**2>=0.935
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-1.25	1.65	1.44	0.39
2 (Bis-H3)	-91.86	98.03	94.89	6.17

D23	2.5752 eV	481.45 nm	f=0.0002	<S**2>=0.804
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-0.7	1.67	1.08	0.97
2 (Bis-H3)	-92.01	98.01	94.96	6

D24	2.5812 eV	480.34 nm	f=0.0003	<S**2>=0.821
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-44.5	2.05	9.55	-42.45
2 (Bis-H3)	-54.77	97.65	73.13	42.88

D25	2.5943 eV	477.91 nm	f=0.0886	<S**2>=1.345
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-4.03	1.47	2.43	-2.56
2 (Bis-H3)	-94.65	98.15	96.39	3.5

D26	2.6211 eV	473.02 nm	f=0.2769	<S**2>=1.243
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-12.46	1.88	4.84	-10.58
2 (Bis-H3)	-87.3	97.68	92.34	10.38

D27	2.6539 eV	467.17 nm	f=0.2235	<S**2>=1.189
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-6.69	1.61	3.28	-5.09
2 (Bis-H3)	-92.98	97.99	95.45	5.02

D28	2.7214 eV	455.6 nm	f=0.9911	<S**2>=1.371
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-3.06	1.6	2.21	-1.46
2 (Bis-H3)	-96.53	97.87	97.2	1.34

D29	2.7915 eV	444.15 nm	f=0.0004	<S**2>=0.808
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-0.02	1.5	0.19	1.48
2 (Bis-H3)	-99.98	98.17	99.07	-1.81

D30	2.8558 eV	434.15 nm	f=0.2404	<S**2>=0.956
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-1.65	1.47	1.56	-0.18
2 (Bis-H3)	-96.69	98.1	97.39	1.41

D31	2.8916 eV	428.77 nm	f=0.0559	<S**2>=1.094
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-38.69	2.15	9.11	-36.54
2 (Bis-H3)	-60.28	97.51	76.67	37.23

D32	2.8953 eV	428.23 nm	f=0.0800	<S**2>=1.133
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-24.96	1.7	6.52	-23.25
2 (Bis-H3)	-74.36	97.93	85.33	23.57

D33	2.9077 eV	426.39 nm	f=0.0355	<S**2>=1.172
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-13.49	1.57	4.6	-11.92
2 (Bis-H3)	-85.59	98.09	91.63	12.5

D34	2.9316 eV	422.93 nm	f=0.0449	<S**2>=1.319
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-5.44	0.87	2.17	-4.57
2 (Bis-H3)	-91.88	98.71	95.23	6.83

D35	2.9555 eV	419.5 nm	f=0.0107	<S**2>=1.168
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-4.5	0.86	1.96	-3.65
2 (Bis-H3)	-92.35	98.71	95.48	6.36

D36	2.9617 eV	418.62 nm	f=0.0340	<S**2>=1.282
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-8.14	1.15	3.06	-6.99
2 (Bis-H3)	-90.54	98.44	94.41	7.9

D37	3.0036 eV	412.79 nm	f=0.0573	<S**2>=1.272
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-10.96	1.47	4.01	-9.49
2 (Bis-H3)	-88.61	98.17	93.26	9.56

D38	3.0377 eV	408.15 nm	f=0.0027	<S**2>=1.142
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-0.89	0.65	0.76	-0.24
2 (Bis-H3)	-91.96	98.98	95.41	7.01

D39	3.0842 eV	402 nm	f=0.0071	<S**2>=1.092
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-1.13	0.68	0.88	-0.45
2 (Bis-H3)	-91.9	98.87	95.32	6.97

D40	3.0901 eV	401.23 nm	f=0.0006	<S**2>=1.045
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-4.39	1.62	2.67	-2.77
2 (Bis-H3)	-86.67	98.02	92.17	11.36

D41	3.166 eV	391.61 nm	f=0.1166	<S**2>=1.210
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-9.54	2.47	4.85	-7.08
2 (Bis-H3)	-89.95	97.08	93.44	7.13

D42	3.2055 eV	386.79 nm	f=0.0210	<S**2>=1.281
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-11.29	1.55	4.18	-9.73
2 (Bis-H3)	-87.16	98.05	92.44	10.89

D43	3.2665 eV	379.56 nm	f=0.0788	<S**2>=1.072
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-6.8	1.53	3.23	-5.27
2 (Bis-H3)	-92.32	98.06	95.15	5.75

D44	3.2864 eV	377.26 nm	f=0.0563	<S**2>=1.320
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-9.54	1.9	4.26	-7.64
2 (Bis-H3)	-89.95	97.69	93.74	7.73

D45	3.3495 eV	370.16 nm	f=0.0428	<S**2>=1.284
Fragment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-9.88	1.34	3.64	-8.54
2 (Bis-H3)	-89.58	98.14	93.76	8.56

Fig.S12: Fragment analysis of 45 doublet excited states' electron-hole distribution of **Mono-Pd** in DCM based on TD-DFT calculation, here positive value indicates gain of electron density and negative value indicates loss of electron density.

D1	0.9494 eV	1305.92 nm	f=0.3617	<S**2>=0.818
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-0.96	1.67	1.27	0.71
2 (Cu)	-1.6	0.13	0.46	-1.47
3 (Bis-H3)	-93.25	97.64	95.42	4.39

D2	1.0377 eV	1194.8 nm	f=0.0001	<S**2>=0.818
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-19.84	1.89	6.12	-17.95
2 (Cu)	-0.01	0.15	0.04	0.14
3 (Bis-H3)	-79.98	97.34	88.24	17.36

D3	1.1043 eV	1122.78 nm	f=0.0072	<S**2>=1.004
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-1.33	3.72	2.22	2.39
2 (Cu)	-0.48	0.16	0.28	-0.33
3 (Bis-H3)	-96.79	94.75	95.77	-2.04

D4	1.4017 eV	884.5 nm	f=0.0007	<S**2>=0.813
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-72.84	2.34	13.05	-70.5
2 (Cu)	0	0.14	0.03	0.14
3 (Bis-H3)	-27.12	96.93	51.27	69.82

D5	1.4097 eV	879.5 nm	f=0.0005	<S**2>=0.823
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-28.63	1.92	7.41	-26.71
2 (Cu)	-0.29	0.14	0.2	-0.14
3 (Bis-H3)	-70.45	97.34	82.81	26.9

D6	1.4694 eV	843.79 nm	f=0.0307	<S**2>=0.817
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-0.38	1	0.62	0.62
2 (Cu)	-1.42	0.59	0.92	-0.83
3 (Bis-H3)	-94.37	94.45	94.41	0.08

D7	1.6368 eV	757.48 nm	f=0.0111	<S**2>=0.828
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-1.27	1.67	1.46	0.4
2 (Cu)	-0.25	0.22	0.23	-0.03
3 (Bis-H3)	-96.8	97.07	96.93	0.27

D8	2.029 eV	611.07 nm	f=0.0021	<S**2>=1.134
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-0.15	0.01	0.04	-0.13
2 (Cu)	-2.23	32.28	8.49	30.04
3 (Bis-H3)	-92.42	46.94	65.87	-45.49

D9	2.0674 eV	599.71 nm	f=0.0005	<S**2>=0.980
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-10.01	1.94	4.41	-8.07
2 (Cu)	-0.59	0.17	0.31	-0.43
3 (Bis-H3)	-84.04	97.22	90.39	13.19

D10	2.0717 eV	598.46 nm	f=0.0177	<S**2>=0.926
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-13.65	1.77	4.92	-11.87
2 (Cu)	-0.44	0.17	0.27	-0.28
3 (Bis-H3)	-85.36	97.26	91.11	11.9

D11	2.1233 eV	583.91 nm	f=0.0037	<S**2>=0.879
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-7.19	1.81	3.61	-5.38
2 (Cu)	-0.58	0.18	0.32	-0.4
3 (Bis-H3)	-86.04	97.21	91.45	11.17

D12	2.1375 eV	580.05 nm	f=0.0010	<S**2>=0.863
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-3.53	1.8	2.52	-1.72
2 (Cu)	-0.07	0.15	0.1	0.08
3 (Bis-H3)	-90.59	97.39	93.93	6.8

D13	2.1377 eV	579.99 nm	f=0.0003	<S**2>=0.925
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-5.61	1.91	3.27	-3.7
2 (Cu)	-0.03	0.14	0.07	0.11
3 (Bis-H3)	-88.87	97.22	92.95	8.35

D14	2.1735 eV	570.45 nm	f=0.1834	<S**2>=1.067
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-15.31	3.14	6.93	-12.18
2 (Cu)	-0.06	0.2	0.11	0.14
3 (Bis-H3)	-84.12	94.82	89.31	10.7

D15	2.2743 eV	545.16 nm	f=0.0022	<S**2>=1.171
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-61.1	4.13	15.89	-56.97
2 (Cu)	-0.05	0.09	0.06	0.04
3 (Bis-H3)	-38.55	94.55	60.37	56

D16	2.2827 eV	543.15 nm	f=0.1348	<S**2>=1.035
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-1.08	3.03	1.81	1.95
2 (Cu)	-1.47	0.27	0.63	-1.21
3 (Bis-H3)	-93.54	95.11	94.32	1.57

D17	2.3254 eV	533.17 nm	f=0.0001	<S**2>=0.814
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	0.01	1.72	0	1.74
2 (Cu)	0	0.15	0.01	0.14
3 (Bis-H3)	-92.5	97.52	94.98	5.01

D18	2.3264 eV	532.94 nm	f=0.0005	<S**2>=0.816
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-0.07	1.72	0.34	1.66
2 (Cu)	0	0.14	0.02	0.14
3 (Bis-H3)	-92.47	97.52	94.96	5.05

D19	2.4614 eV	503.71 nm	f=0.0083	<S**2>=0.840
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-0.14	1.69	0.49	1.54
2 (Cu)	-0.18	0.16	0.17	-0.02
3 (Bis-H3)	-93.44	97.52	95.46	4.09

D20	2.4685 eV	502.26 nm	f=0.0014	<S**2>=0.819
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-0.04	1.7	0.26	1.66
2 (Cu)	-0.11	0.15	0.12	0.04
3 (Bis-H3)	-93.61	97.56	95.57	3.95

D21	2.5352 eV	489.05 nm	f=0.1547	<S**2>=0.883
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-17.84	2.65	6.87	-15.19
2 (Cu)	-0.34	0.13	0.21	-0.21
3 (Bis-H3)	-79.54	96.25	87.5	16.7

D22	2.5777 eV	480.99 nm	f=0.0028	<S**2>=0.816
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-44.89	2.08	9.67	-42.8
2 (Cu)	0	0.14	0	0.14
3 (Bis-H3)	-54.49	97.18	72.77	42.69

D23	2.5855 eV	479.53 nm	f=0.0068	<S**2>=0.811
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-0.08	1.71	0.37	1.63
2 (Cu)	-0.01	0.15	0.03	0.14
3 (Bis-H3)	-92.51	97.54	94.99	5.02

D24	2.5869 eV	479.28 nm	f=0.0014	<S**2>=0.803
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	0.02	1.7	0	1.72
2 (Cu)	-0.02	0.15	0.05	0.13
3 (Bis-H3)	-92.68	97.58	95.1	4.9

D25	2.6137 eV	474.37 nm	f=0.0112	<S**2>=0.871
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-15.03	1.57	4.86	-13.46
2 (Cu)	-0.1	0.54	0.24	0.43
3 (Bis-H3)	-84.04	94.66	89.19	10.61

D26	2.769 eV	447.76 nm	f=0.0172	<S**2>=1.208
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-1.39	0.14	0.44	-1.25
2 (Cu)	-1.06	28.92	5.55	27.86
3 (Bis-H3)	-96.46	52	70.82	-44.46

D27	2.7877 eV	444.76 nm	f=0.3047	<S**2>=1.249
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-2.92	1.76	2.27	-1.16
2 (Cu)	-0.87	1.38	1.1	0.5
3 (Bis-H3)	-91.59	93	92.29	1.41

D28	2.7959 eV	443.45 nm	f=0.0008	<S**2>=0.814
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-0.01	1.51	0.1	1.51
2 (Cu)	0	0.14	0.02	0.13
3 (Bis-H3)	-99.99	97.76	98.87	-2.24

D29	2.8221 eV	439.34 nm	f=0.6841	<S**2>=1.257
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-4.28	1.48	2.52	-2.8
2 (Cu)	-0.71	1.51	1.04	0.8
3 (Bis-H3)	-92.52	94.59	93.55	2.07

D30	2.8674 eV	432.39 nm	f=0.2298	<S**2>=1.284
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-1.48	1.41	1.45	-0.07
2 (Cu)	-1.09	1.03	1.06	-0.06
3 (Bis-H3)	-93.95	93.82	93.89	-0.14

D31	2.8792 eV	430.61 nm	f=0.0047	<S**2>=0.915
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-0.01	0.57	0.08	0.56
2 (Cu)	-0.29	0.76	0.47	0.47
3 (Bis-H3)	-93.51	94.07	93.79	0.56

D32	2.8855 eV	429.68 nm	f=0.0038	<S**2>=1.091
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-1.84	1.06	1.4	-0.78
2 (Cu)	-0.14	0.6	0.29	0.46
3 (Bis-H3)	-92.25	94.33	93.29	2.08

D33	2.9116 eV	425.83 nm	f=0.1253	<S**2>=1.334
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-14.91	1.37	4.51	-13.54
2 (Cu)	-0.5	0.66	0.58	0.16
3 (Bis-H3)	-83.2	95.58	89.17	12.38

D34	2.9494 eV	420.37 nm	f=0.0448	<S**2>=1.314
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-3.9	1.38	2.31	-2.52
2 (Cu)	-1.08	0.52	0.75	-0.57
3 (Bis-H3)	-93.19	96.1	94.63	2.92

D35	2.9699 eV	417.47 nm	f=0.0124	<S**2>=0.864
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-1.51	0.07	0.33	-1.44
2 (Cu)	-5.1	30.12	12.4	25.02
3 (Bis-H3)	-80.81	49.97	63.55	-30.83

D36	3.0658 eV	404.41 nm	f=0.0004	<S**2>=1.249
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-1.43	0.69	0.99	-0.75
2 (Cu)	0.01	0.71	0	0.72
3 (Bis-H3)	-91.48	94.52	92.99	3.04

D37	3.0668 eV	404.27 nm	f=0.0001	<S**2>=1.243
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-0.1	0.63	0.25	0.53
2 (Cu)	0	0.72	0.05	0.71
3 (Bis-H3)	-92.47	93.67	93.06	1.2

D38	3.091 eV	401.11 nm	f=0.0146	<S**2>=1.140
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-19.8	1.38	5.22	-18.42
2 (Cu)	-1.74	1.57	1.65	-0.16
3 (Bis-H3)	-76.56	93.37	84.55	16.81

D39	3.094 eV	400.72 nm	f=0.0412	<S**2>=1.231
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-2.87	1.65	2.18	-1.22
2 (Cu)	-0.58	0.74	0.65	0.16
3 (Bis-H3)	-94.25	95.17	94.71	0.92

D40	3.1309 eV	396.01 nm	f=0.0002	<S**2>=0.831
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-0.03	1.68	0.24	1.64
2 (Cu)	-0.14	0.21	0.17	0.08
3 (Bis-H3)	-88.12	97.52	92.7	9.4

D41	3.1464 eV	394.05 nm	f=0.0025	<S**2>=1.280
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-2.6	1.83	2.19	-0.77
2 (Cu)	-0.91	0.54	0.7	-0.37
3 (Bis-H3)	-92.31	95.38	93.83	3.07

D42	3.163 eV	391.98 nm	f=0.0002	<S**2>=1.039
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-8.29	1.86	3.93	-6.43
2 (Cu)	-2.78	2.03	2.37	-0.75
3 (Bis-H3)	-85.88	94.1	89.9	8.21

D43	3.1822 eV	389.62 nm	f=0.1603	<S**2>=1.263
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-10.01	3.1	5.57	-6.91
2 (Cu)	-1.2	1.7	1.43	0.5
3 (Bis-H3)	-86.54	92.51	89.48	5.97

D44	3.249 eV	381.61 nm	f=0.0186	<S**2>=1.044
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-20.37	1.58	5.68	-18.78
2 (Cu)	-1.31	3.95	2.27	2.64
3 (Bis-H3)	-77.51	91.04	84	13.53

D45	3.2959 eV	376.17 nm	f=0.0176	<S**2>=1.339
Frgment	Hole/%	Electron/%	Overlap/%	Diff/%
1 (Pd)	-5.56	2.73	3.89	-2.83
2 (Cu)	-1.69	2.55	2.08	0.87
3 (Bis-H3)	-88.93	88.64	88.79	-0.28

Fig.S13: Fragment analysis of 45 Doublet excited states' electron-hole distribution of **Mix-Cu-Pd** in DCM based on TD-DFT calculation, here positive value indicates gain of electron density and negative value indicates loss of electron density.

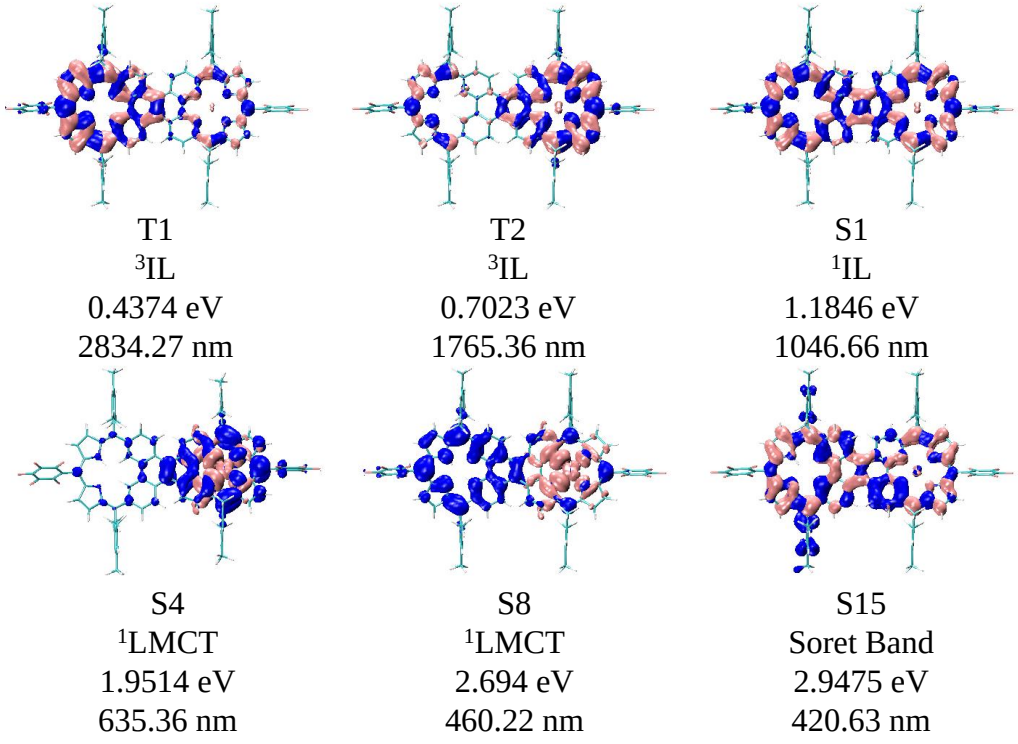
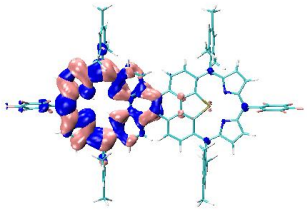
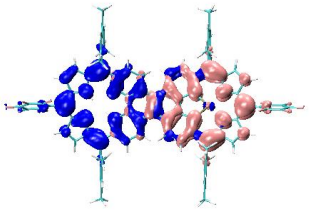


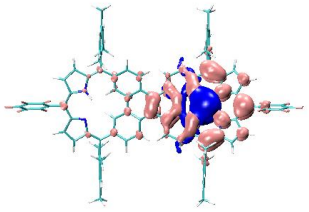
Fig.S14: Electron-hole density distribution of selected excited states of **Mono-Cu** in DCM based on TD-DFT calculation results. Here blue indicates loss of electron density (hole) and pink indicates gain of electron density compared with ground state.



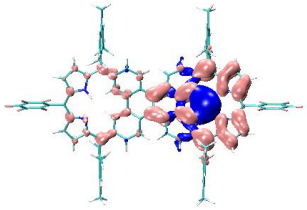
ES1 Q1
^{4}IL
0.5372 eV
2308.01 nm



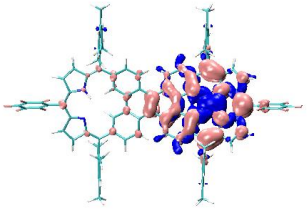
ES2 D1
^{2}ILCT
0.8748 eV
1417.28 nm



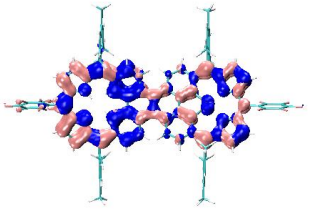
ES6 D5
^{2}MLCT
1.4059 eV
881.88 nm



ES23 D16
^{2}MLCT
2.2687 eV
546.49 nm



ES37 D24
^{2}MLCT
2.5812 eV
480.34 nm



ES41 D28
Soret Band
2.7214 eV
455.6 nm

Fig.S15: Electron-hole density distribution of selected excited states of **Mono-Pd** in DCM based on TD-DFT calculation results. Here blue indicates loss of electron density (hole) and pink indicates gain of electron density compared with ground state.

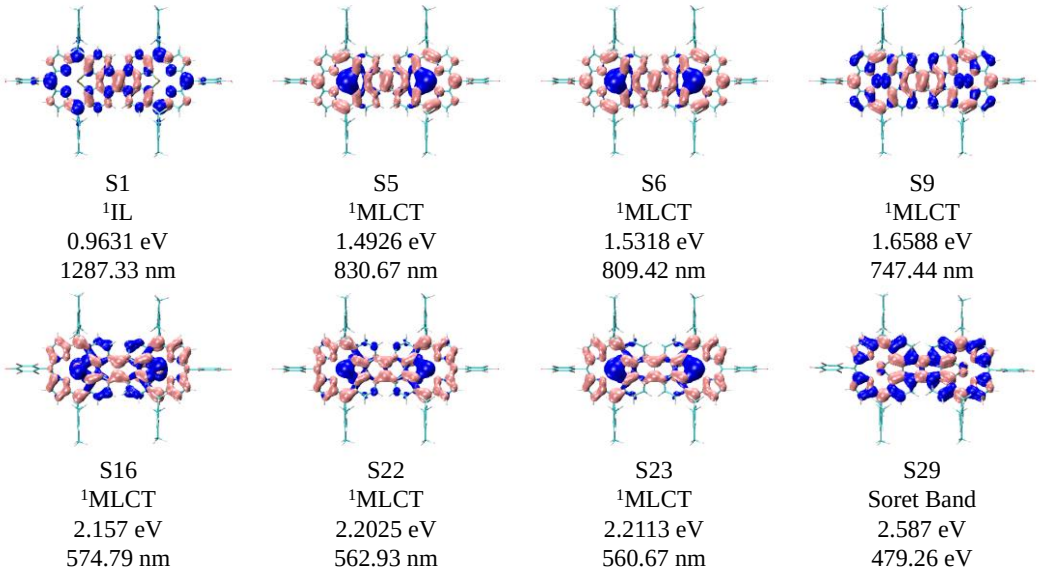


Fig.S16: Electron-hole density distribution of selected excited states of **Bis-Pd** in DCM based on TD-DFT calculation results. Here blue indicates loss of electron density (hole) and pink indicates gain of electron density compared with ground state.

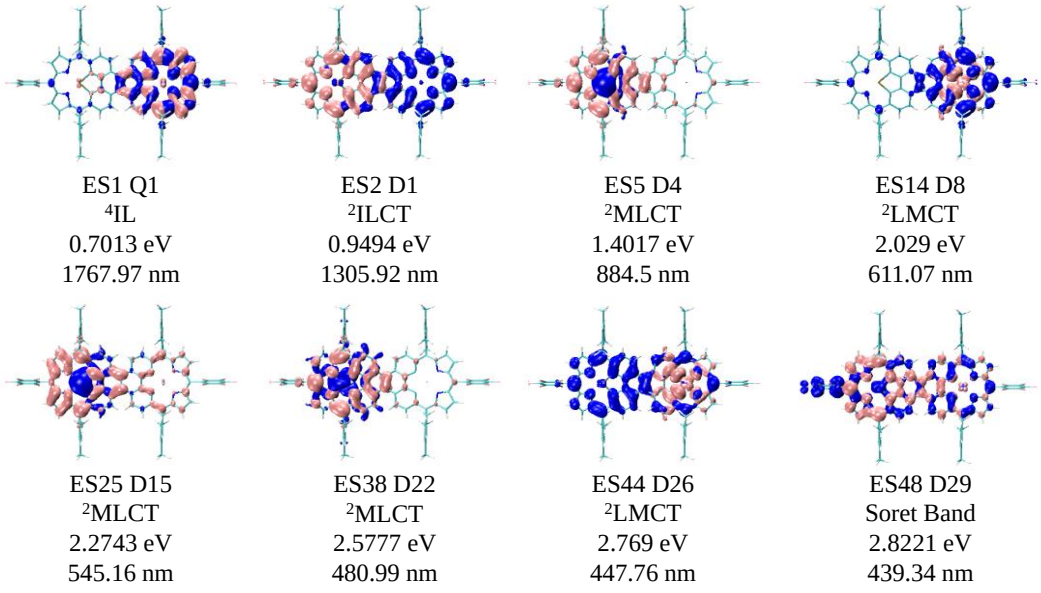
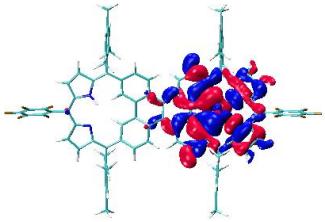


Fig.S17: Electron-hole density distribution of selected excited states of **Mix-Cu-Pd** in DCM based on TD-DFT calculation results. Here blue indicates loss of electron density (hole) and pink indicates gain of electron density compared with ground state.



LUMO+2

Fig.S18: Shape of molecular orbital with d-orbital component correlates with excited states in the first 48 singlet excited states of **Mono-Cu** extracted by TD-DFT calculation.

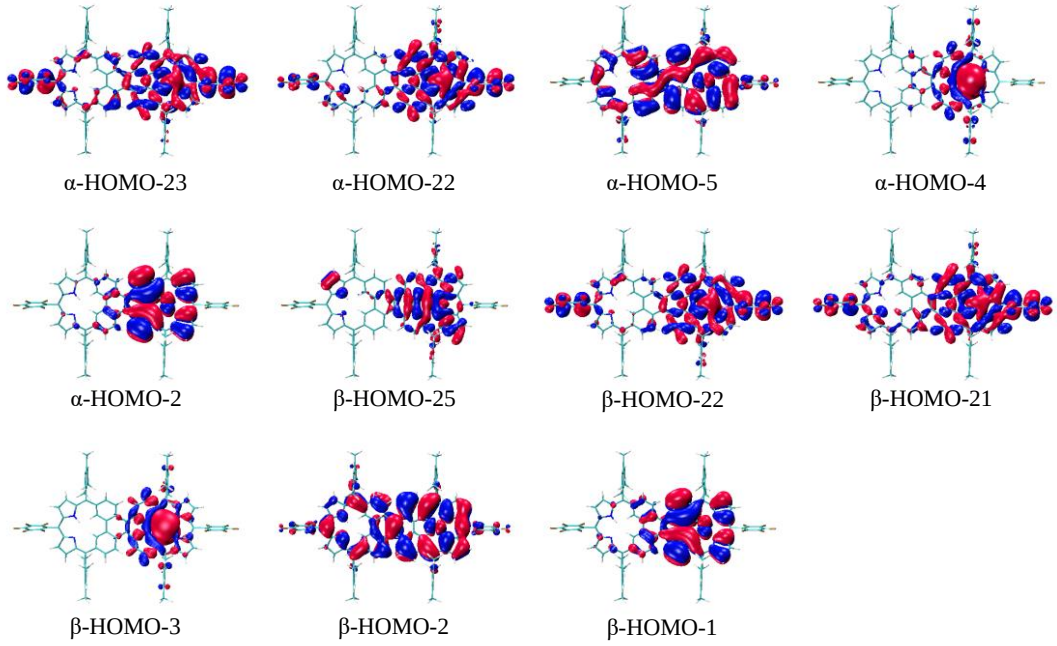


Fig.S19: Shape of molecular orbitals with d-orbital component correlate with excited states in the first 96 excited states of **Mono-Pd** extracted by TD-DFT calculation.

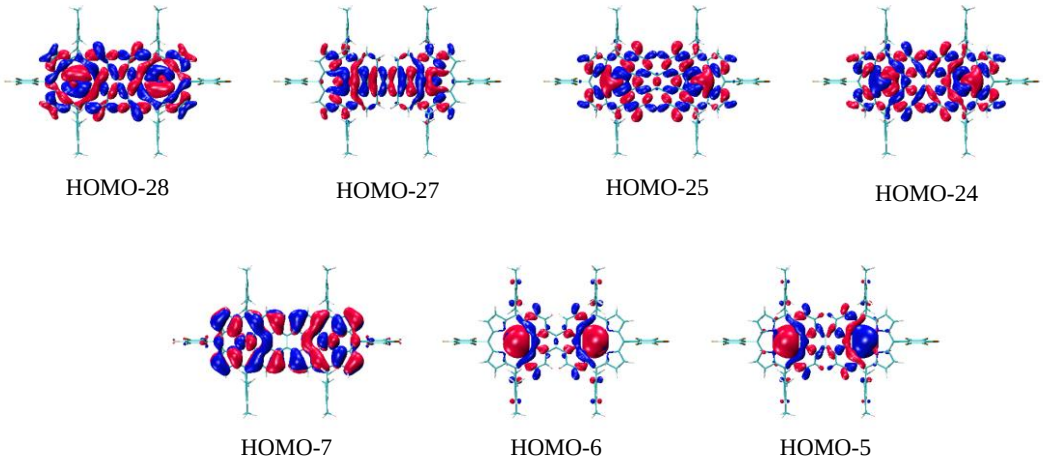


Fig.S20: Shape of molecular orbitals with d-orbital component correlate with excited states in the first 48 singlet excited states of **Bis-Pd** extracted by TD-DFT calculation.

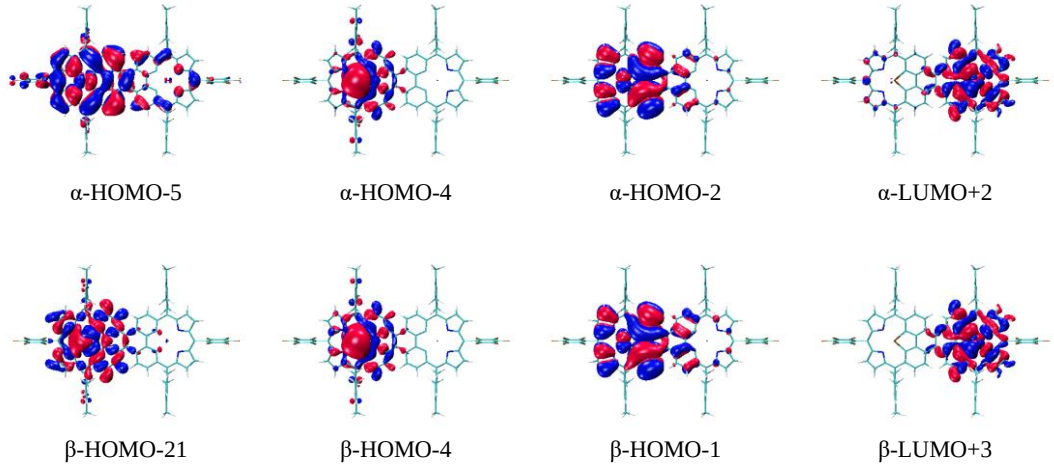


Fig.S21: Shape of molecular orbitals with d-orbital component correlate with excited states in the first 96 excited states of **Mix-Cu-Pd** extracted by TD-DFT calculation.

Cartesian Co-ordinates (XYZ format) of S0 state of Bis-Pd.			
C96H60F10N4Pd2			
C	-3.8029	-2.6393	-0.6829
C	-3.7187	-1.2686	-0.3303
C	-2.4371	-0.6981	-0.1668
C	-1.2337	-1.4217	-0.2666
C	-1.3473	-2.7806	-0.7009

C	-2.5761	-3.3545	-0.9034
C	-2.4371	0.6978	0.1662
C	-1.2338	1.4215	0.2659
C	-0.0001	0.7286	-0.0005
C	-0.0001	-0.7288	-0.0004
C	-3.8029	2.639	0.6827
C	-2.5761	3.3542	0.903
C	-1.3472	2.7803	0.7003
C	1.2335	1.4215	-0.267
C	2.4369	0.6979	-0.1673
C	2.437	-0.6981	0.1659
C	1.2336	-1.4217	0.2658
C	3.7185	-1.2685	0.3295
C	3.8028	-2.6391	0.6824
C	2.5761	-3.3543	0.9031
C	1.3472	-2.7805	0.7004
C	1.347	2.7803	-0.7014
C	2.5758	3.3542	-0.9041
C	3.8026	2.6391	-0.6836
C	3.7184	1.2684	-0.3309
C	-5.0604	-3.3083	-0.8411
C	-6.3241	-2.7146	-0.6793
C	-5.0604	3.3078	0.8412
C	-6.3241	2.7141	0.6795
C	5.0601	3.308	-0.8418
C	5.0604	-3.3079	0.8408
C	6.324	-2.7142	0.6791
C	6.3238	2.7144	-0.6798
C	-7.5942	-3.4063	-0.8087
C	-8.5733	-2.4911	-0.5703
C	-7.9122	-1.2245	-0.2988
N	-6.5743	-1.4076	-0.3694
N	-6.5743	1.4071	0.3698
C	-7.9122	1.224	0.2993
C	-8.5733	2.4906	0.5705
C	-7.5941	3.4059	0.8086
C	7.5938	3.4064	-0.8087
C	8.573	2.4912	-0.5702
C	7.912	1.2245	-0.2992
N	6.5741	1.4074	-0.3701
N	6.5742	-1.4072	0.3693
C	7.9121	-1.224	0.2989
C	8.5732	-2.4906	0.5701

C	7.5941	-3.4059	0.8084
C	8.5536	0.0003	-0.0001
C	-8.5537	-0.0003	0.0003
C	10.0377	0.0004	0.0002
C	5.0571	-4.756	1.1983
C	5.0568	4.7563	-1.1987
C	-5.0571	-4.7564	-1.1985
C	-5.0571	4.756	1.1985
C	-10.0379	-0.0003	0.0003
C	-10.7625	-0.1901	-1.1788
C	-12.154	-0.1926	-1.1902
C	-12.8501	-0.0001	0.0005
C	-12.1539	0.1924	1.1911
C	-10.7624	0.1896	1.1796
C	10.7625	0.1905	-1.1789
C	12.154	0.1933	-1.19
C	12.85	0.0007	0.0007
C	12.1536	-0.192	1.1912
C	10.7621	-0.1896	1.1795
C	4.9811	-5.7247	0.1808
C	4.9731	-7.0751	0.5386
C	5.0362	-7.486	1.8733
C	5.1044	-6.5017	2.863
C	5.1174	-5.1397	2.5502
C	4.986	5.7244	-0.1805
C	4.9862	7.0753	-0.5371
C	5.0487	7.4869	-1.8716
C	5.1189	6.503	-2.8617
C	5.1235	5.1408	-2.5501
C	-5.1167	5.1398	2.5504
C	-5.1037	6.5018	2.8631
C	-5.0361	7.486	1.8733
C	-4.9736	7.075	0.5386
C	-4.9817	5.7245	0.1809
C	-5.117	-5.1403	-2.5503
C	-5.104	-6.5023	-2.8629
C	-5.036	-7.4865	-1.8731
C	-4.9733	-7.0754	-0.5385
C	-4.9815	-5.7249	-0.1809
C	-5.0574	8.9438	2.2307
C	-4.9095	5.312	-1.2608
C	-5.1844	4.1042	3.6354
C	-5.1848	-4.1048	-3.6354

C	-5.0575	-8.9443	-2.2306
C	-4.9091	-5.3123	1.2609
C	4.9082	-5.3122	-1.2609
C	5.0576	-8.9439	2.2308
C	5.1857	-4.1041	3.6351
C	5.1978	4.1058	-3.6352
C	5.0114	8.9437	-2.2319
C	4.9179	5.3114	1.2613
F	10.1257	-0.3668	2.3269
F	12.8164	-0.3687	2.3212
F	14.1691	0.0009	0.001
F	12.8172	0.3702	-2.3197
F	10.1266	0.3677	-2.3265
F	-10.1264	-0.3672	-2.3264
F	-10.1261	0.3666	2.3271
H	-0.4526	-3.358	-0.93
H	-2.6264	-4.386	-1.2583
H	-2.6264	4.3856	1.258
H	-0.4525	3.3577	0.9293
H	2.6264	-4.3857	1.2581
H	0.4525	-3.3579	0.9296
H	0.4523	3.3576	-0.9305
H	2.6262	4.3856	-1.2591
H	-7.7096	-4.4621	-1.0447
H	-9.6482	-2.6601	-0.5672
Pd	5.177	0	-0.0006
H	-9.6482	2.6596	0.5674
H	-7.7096	4.4618	1.0445
H	7.7092	4.4622	-1.0444
H	9.6479	2.6604	-0.5667
H	9.6482	-2.6596	0.567
H	7.7096	-4.4617	1.0443
F	-12.8171	-0.3692	-2.3201
F	-14.1693	0	0.0006
F	-12.8168	0.3691	2.321
H	4.9133	-7.8288	-0.2523
H	5.1458	-6.8008	3.9146
H	4.9377	7.8287	0.2547
H	5.1726	6.8029	-3.9126
H	-5.1447	6.8009	3.9147
H	-4.9143	7.8287	-0.2524
H	-5.1452	-6.8015	-3.9145
H	-4.9138	-7.829	0.2525

H	-4.4868	9.5445	1.5077
H	-6.0899	9.3316	2.233
H	-4.6412	9.1194	3.2331
H	-4.0286	4.6786	-1.4513
H	-5.7911	4.7192	-1.5517
H	-4.8514	6.187	-1.9221
H	-6.0975	3.4939	3.5494
H	-4.3341	3.4066	3.576
H	-5.1774	4.5699	4.6301
H	-6.0977	-3.4943	-3.5492
H	-4.3343	-3.4074	-3.5762
H	-5.1782	-4.5705	-4.63
H	-4.6348	-9.1206	-3.2301
H	-4.4929	-9.5459	-1.5037
H	-6.0907	-9.3302	-2.2401
H	-4.0286	-4.6783	1.4511
H	-5.791	-4.7201	1.552
H	-4.8503	-6.1873	1.9221
H	4.8501	-6.1873	-1.9221
H	4.0272	-4.679	-1.4511
H	5.7896	-4.7193	-1.5522
H	6.0899	-9.3321	2.2305
H	4.6437	-9.1191	3.2341
H	4.485	-9.5442	1.5091
H	4.3358	-3.4059	3.5756
H	5.1783	-4.5697	4.6298
H	6.0991	-3.4944	3.5492
H	6.1132	3.4992	-3.5477
H	4.3502	3.4049	-3.5776
H	5.1909	4.5717	-4.6298
H	5.4668	9.5648	-1.4472
H	3.9717	9.2892	-2.3585
H	5.5367	9.1387	-3.1779
H	4.0388	4.6761	1.4534
H	5.8014	4.7204	1.5503
H	4.8594	6.1861	1.9229
C	-3.7186	1.2683	0.33
Pd	-5.1772	-0.0002	0.0001

Cartesian Co-ordinates (XYZ format) of S0 state of Mix-Cu-Pd.			
C96H60CuF10N4Pd			
C	3.9479	2.6035	-0.6467

C	3.8589	1.2513	-0.3004
C	2.5756	0.6946	-0.1417
C	1.3732	1.4167	-0.2254
C	1.4904	2.7641	-0.6461
C	2.7305	3.3208	-0.8499
C	2.5756	-0.6945	0.141
C	1.3732	-1.4167	0.2245
C	0.117	-0.7129	-0.0084
C	0.117	0.7129	0.0073
C	3.9479	-2.6033	0.6462
C	2.7305	-3.3206	0.8492
C	1.4904	-2.764	0.6452
C	-1.1219	-1.4209	-0.2505
C	-2.3246	-0.6975	-0.1569
C	-2.3246	0.6975	0.1557
C	-1.122	1.4209	0.2494
C	-3.6121	1.2712	0.3202
C	-3.6976	2.6364	0.6667
C	-2.4718	3.3531	0.8808
C	-1.2413	2.7807	0.6775
C	-1.2413	-2.7806	-0.6786
C	-2.4717	-3.3531	-0.8819
C	-3.6976	-2.6365	-0.6677
C	-3.6121	-1.2712	-0.3214
C	5.1954	3.3104	-0.8267
C	6.4081	2.6953	-0.669
C	5.1955	-3.3102	0.8264
C	6.4082	-2.6949	0.669
C	-4.959	-3.31	-0.8248
C	-4.9591	3.3099	0.8241
C	-6.2238	2.7219	0.6667
C	-6.2237	-2.722	-0.6672
C	7.6831	3.37	-0.8006
C	8.6482	2.4521	-0.5623
C	7.9762	1.1938	-0.2892
N	6.6311	1.361	-0.3527
N	6.6311	-1.3606	0.3527
C	7.9762	-1.1933	0.2896
C	8.6483	-2.4516	0.5628
C	7.6831	-3.3696	0.8009
C	-7.4925	-3.4129	-0.7946
C	-8.4723	-2.4953	-0.5608
C	-7.81	-1.2304	-0.2947

N	-6.4735	-1.4119	-0.3626
N	-6.4736	1.4118	0.3619
C	-7.81	1.2301	0.2945
C	-8.4724	2.4949	0.5611
C	-7.4926	3.4126	0.7947
C	-8.4522	-0.0002	0
C	8.6474	0.0002	0.0003
C	-9.9358	-0.0003	0.0002
C	-4.9511	4.7587	1.1771
C	-4.951	-4.759	-1.1772
C	5.1752	4.7564	-1.1849
C	5.1752	-4.7562	1.1846
C	10.1293	0.0003	0.0005
C	10.8566	0.1704	-1.1802
C	12.2483	0.1765	-1.192
C	12.9447	0.0004	0.0009
C	12.2479	-0.1757	1.1935
C	10.8563	-0.1697	1.1813
C	-10.6602	-0.193	-1.1786
C	-12.0517	-0.1957	-1.1897
C	-12.7476	-0.0005	0.0007
C	-12.0513	0.1948	1.1908
C	-10.6599	0.1923	1.1792
C	-4.8774	5.7238	0.1563
C	-4.8645	7.0751	0.5105
C	-4.9205	7.4898	1.8444
C	-4.9866	6.5083	2.837
C	-5.0043	5.1455	2.5282
C	-4.8824	-5.7236	-0.1557
C	-4.8779	-7.0753	-0.5089
C	-4.9334	-7.4907	-1.8424
C	-5.0015	-6.5097	-2.8355
C	-5.0108	-5.1466	-2.5279
C	5.2033	-5.1403	2.5376
C	5.1719	-6.5017	2.8519
C	5.1147	-7.4866	1.8621
C	5.0826	-7.0767	0.5259
C	5.1109	-5.7267	0.1676
C	5.2035	5.1406	-2.5379
C	5.1721	6.502	-2.8522
C	5.1146	7.4868	-1.8623
C	5.0822	7.077	-0.5262
C	5.1105	5.7269	-0.1679

C	5.1146	-8.9441	2.2214
C	5.0738	-5.316	-1.2759
C	5.2614	-4.1049	3.6234
C	5.262	4.1052	-3.6236
C	5.1145	8.9443	-2.2219
C	5.0731	5.3163	1.2756
C	-4.8119	5.3067	-1.2844
C	-4.9368	8.9486	2.198
C	-5.0701	4.1127	3.616
C	-5.0828	-4.1145	-3.6159
C	-4.8909	-8.9484	-2.1986
C	-4.8216	-5.3058	1.285
F	-10.0229	0.3722	2.3258
F	-12.7142	0.374	2.3203
F	-14.0667	-0.0006	0.0009
F	-12.7149	-0.375	-2.319
F	-10.0236	-0.3728	-2.3254
F	10.2208	0.3349	-2.3306
F	10.2202	-0.3343	2.3316
H	0.6059	3.3614	-0.86
H	2.7991	4.3566	-1.1878
H	2.7991	-4.3565	1.1871
H	0.606	-3.3613	0.859
H	-2.5211	4.3869	1.2296
H	-0.352	3.3665	0.9033
H	-0.3519	-3.3665	-0.9044
H	-2.5212	-4.3869	-1.2306
H	7.7973	4.4256	-1.0385
H	9.7258	2.5997	-0.5561
Pd	-5.0714	0	-0.0006
H	9.7258	-2.5991	0.5569
H	7.7973	-4.4251	1.0388
H	-7.6089	-4.4696	-1.0266
H	-9.5474	-2.6633	-0.5582
H	-9.5475	2.6627	0.5589
H	-7.609	4.4691	1.0269
F	12.9116	0.3394	-2.3246
F	14.2647	0.0005	0.0011
F	12.911	-0.3386	2.3263
H	-4.8063	7.8264	-0.2827
H	-5.0225	6.8103	3.888
H	-4.8308	-7.8264	0.2853
H	-5.0497	-6.8125	-3.8858

H	5.189	-6.8002	3.9044
H	5.031	-7.8309	-0.2651
H	5.1894	6.8004	-3.9047
H	5.0303	7.8312	0.2647
H	4.5518	-9.5399	1.4884
H	6.143	-9.3422	2.2435
H	4.6779	-9.1142	3.2159
H	4.2255	-4.6434	-1.4787
H	5.985	-4.7649	-1.5572
H	4.9841	-6.1896	-1.9357
H	6.1967	-3.5253	3.5727
H	4.4378	-3.3798	3.5296
H	5.2001	-4.5679	4.6175
H	6.1973	3.5256	-3.5727
H	4.4384	3.38	-3.5301
H	5.2009	4.5682	-4.6178
H	4.6718	9.115	-3.2137
H	4.5573	9.5411	-1.4854
H	6.1434	9.3407	-2.2508
H	4.2247	4.6436	1.4782
H	5.9842	4.7652	1.5572
H	4.9832	6.1898	1.9354
H	-4.7497	6.1792	-1.9484
H	-3.936	4.6665	-1.475
H	-5.6985	4.7192	-1.571
H	-5.9682	9.3394	2.2015
H	-4.5178	9.1256	3.1989
H	-4.3661	9.5457	1.4721
H	-4.2235	3.4111	3.5527
H	-5.0547	4.5806	4.6095
H	-5.9867	3.5068	3.5369
H	-6.0013	-3.5117	-3.5353
H	-4.2384	-3.41	-3.5546
H	-5.0678	-4.5828	-4.6093
H	-5.3487	-9.5685	-1.4144
H	-3.8498	-9.2918	-2.3194
H	-5.4113	-9.1472	-3.1465
H	-3.9479	-4.6633	1.4773
H	-5.7105	-4.7206	1.5694
H	-4.7587	-6.178	1.9495
C	3.8589	-1.2511	0.2998
Cu	5.314	0.0001	-0.0001

Cartesian Co-ordinates (XYZ format) of S0 state of Mono-Cu			
C96H63CuF10N4			
C	-3.9569	-2.589	-1.0516
C	-3.8469	-1.2111	-0.929
C	-2.628	-0.5672	-0.691
C	-1.4311	-1.3198	-0.5951
C	-1.5301	-2.6999	-0.9139
C	-2.746	-3.323	-1.1166
C	-2.6181	0.847	-0.3839
C	-1.401	1.4961	-0.0936
C	-0.1505	0.7658	-0.2554
C	-0.1803	-0.6423	-0.2698
C	-3.8266	1.5435	-0.2584
C	-3.9184	2.7936	0.337
C	-2.6984	3.4084	0.7198
C	-1.4861	2.7908	0.4823
C	1.122	1.4607	-0.3875
C	2.3063	0.7167	-0.2582
C	2.2656	-0.6702	0.0196
C	1.0456	-1.3696	0.052
C	3.5321	-1.2463	0.2517
C	3.5814	-2.5901	0.6285
C	2.3416	-3.2764	0.7995
C	1.1227	-2.705	0.522
C	1.2809	2.8183	-0.7612
C	2.5384	3.3558	-0.8949
C	3.7338	2.6095	-0.6606
C	3.6065	1.2548	-0.3449
C	-5.2667	-3.2398	-1.0733
C	-6.4693	-2.6404	-0.7473
C	-5.2137	3.4204	0.6029
C	-6.428	2.7715	0.6016
C	5.0021	3.2954	-0.7833
C	4.8072	-3.3207	0.868
C	6.037	-2.7367	0.7386
C	6.1952	2.6526	-0.5997
C	-7.7378	-3.3688	-0.7643
C	-8.6992	-2.4905	-0.3964
C	-8.0184	-1.2136	-0.1632
N	-6.7056	-1.3218	-0.3574
N	-6.7324	1.4236	0.4168
C	-8.0791	1.2104	0.4387
C	-8.6998	2.498	0.6832

C	-7.714	3.4254	0.779
C	7.4886	3.2989	-0.6896
C	8.426	2.3557	-0.4407
C	7.7186	1.11	-0.1983
N	6.38	1.3086	-0.2948
N	6.2996	-1.411	0.4111
C	7.6491	-1.2757	0.3812
C	8.2842	-2.5466	0.6851
C	7.2923	-3.4383	0.9122
C	8.3552	-0.0995	0.1026
C	-8.7059	-0.0089	0.2147
C	9.8362	-0.1335	0.1359
C	4.7404	-4.7591	1.2503
C	5.0218	4.7475	-1.1162
C	-5.2807	-4.6893	-1.4276
C	-5.2103	4.8749	0.9305
C	-10.1818	-0.0467	0.3331
C	-10.9974	-0.2997	-0.7742
C	-12.3843	-0.3449	-0.6743
C	-12.9913	-0.1195	0.5586
C	-12.2084	0.1441	1.6789
C	-10.8222	0.174	1.5561
C	10.5929	0.0221	-1.0284
C	11.9842	-0.0039	-1.0106
C	12.651	-0.198	0.1963
C	11.9249	-0.3596	1.3733
C	10.5344	-0.3211	1.3315
C	4.678	-5.7463	0.2493
C	4.6046	-7.0884	0.6303
C	4.5903	-7.4746	1.9737
C	4.6468	-6.4736	2.9473
C	4.722	-5.1194	2.6101
C	4.9556	5.7011	-0.084
C	4.9719	7.058	-0.418
C	5.0467	7.4905	-1.7449
C	5.1123	6.522	-2.7507
C	5.0996	5.1552	-2.4608
C	-5.3066	5.2992	2.2683
C	-5.2716	6.6702	2.5456
C	-5.1464	7.6253	1.5351
C	-5.046	7.1768	0.2136
C	-5.0707	5.8188	-0.107
C	-5.3119	-5.0702	-2.7824

C	-5.2957	-6.4296	-3.1018
C	-5.2432	-7.4191	-2.1152
C	-5.2026	-7.0136	-0.7791
C	-5.2205	-5.6635	-0.415
C	-5.1339	9.0934	1.8483
C	-4.9613	5.3687	-1.5348
C	-5.4351	4.305	3.3873
C	-5.3714	-4.0296	-3.8628
C	-5.2545	-8.8743	-2.4844
C	-5.1741	-5.2642	1.0319
C	4.6914	-5.3614	-1.2017
C	4.5428	-8.9249	2.3587
C	4.7778	-4.0664	3.6789
C	5.1716	4.1378	-3.5625
C	5.0269	8.953	-2.0834
C	4.8771	5.2661	1.3506
F	9.8709	-0.4714	2.4683
F	12.5597	-0.5392	2.5199
F	13.9706	-0.2286	0.2245
F	12.6753	0.1455	-2.1286
F	9.9861	0.2034	-2.192
F	-10.4517	-0.5017	-1.9647
F	-10.1071	0.4198	2.6446
H	-4.7747	-0.6527	-0.9633
H	-0.6274	-3.2977	-1.0171
H	-2.7722	-4.396	-1.3172
H	-4.724	1.079	-0.6446
H	-2.7192	4.3773	1.2226
H	-0.5788	3.2892	0.8215
H	2.3734	-4.3019	1.1731
H	0.2224	-3.282	0.7225
H	0.4168	3.4402	-0.9906
H	2.6408	4.3992	-1.1996
H	-7.8541	-4.4186	-1.0271
H	-9.7644	-2.6818	-0.2807
H	-6.1131	0.6224	0.3225
Cu	5.0233	-0.025	0.0083
H	-9.7726	2.6672	0.7419
H	-7.8254	4.4967	0.9324
H	7.6331	4.3545	-0.9105
H	9.5063	2.4777	-0.4064
H	9.3578	-2.7196	0.7069
H	7.3758	-4.4928	1.1667

F	-13.1291	-0.5851	-1.7412
F	-14.3072	-0.1538	0.6638
F	-12.7849	0.3549	2.8512
H	4.5543	-7.8553	-0.1485
H	4.6279	-6.7532	4.005
H	4.9255	7.7992	0.3855
H	5.1755	6.8385	-3.7962
H	-5.3389	6.9992	3.5869
H	-4.9446	7.9078	-0.5945
H	-5.3222	-6.7238	-4.1555
H	-5.1509	-7.7708	0.0091
H	-4.3278	9.6118	1.3074
H	-6.0812	9.5687	1.5448
H	-4.9999	9.2754	2.9237
H	-4.0577	4.7587	-1.6935
H	-5.8182	4.7392	-1.8211
H	-4.918	6.2263	-2.2198
H	-6.4245	3.8198	3.384
H	-4.6902	3.4994	3.298
H	-5.3032	4.7916	4.3634
H	-6.2808	-3.415	-3.772
H	-4.5176	-3.3366	-3.7991
H	-5.3655	-4.4901	-4.8601
H	-4.6673	-9.0629	-3.3952
H	-4.8496	-9.499	-1.6756
H	-6.2821	-9.2204	-2.6851
H	-4.3692	-4.5373	1.2227
H	-6.1137	-4.7806	1.3427
H	-5.0102	-6.137	1.6784
H	4.6035	-6.2448	-1.8484
H	3.8631	-4.6758	-1.4409
H	5.6212	-4.8332	-1.4653
H	5.5598	-9.3469	2.4227
H	4.0692	-9.0661	3.3408
H	3.9903	-9.5207	1.6178
H	3.9796	-3.3191	3.5466
H	4.6724	-4.509	4.6786
H	5.7311	-3.5154	3.647
H	6.0939	3.5395	-3.494
H	4.3323	3.4269	-3.5056
H	5.1487	4.6187	-4.5498
H	5.4268	9.5629	-1.2607
H	3.9966	9.297	-2.2748

H	5.6129	9.1649	-2.9894
H	4.0149	4.6019	1.5201
H	5.7732	4.6972	1.6446
H	4.783	6.1292	2.0235

Cartesian Co-ordinates (XYZ format) of S0 state of Mono-Pd			
C96H63F10N4Pd			
C	-4.0779	2.5911	1.047
C	-3.9671	1.2112	0.9261
C	-2.7489	0.5696	0.6913
C	-1.5532	1.3233	0.5976
C	-1.6516	2.7027	0.9171
C	-2.8682	3.3258	1.1164
C	-2.7372	-0.8466	0.3831
C	-1.5193	-1.496	0.0996
C	-0.2671	-0.7709	0.2718
C	-0.2989	0.6526	0.2696
C	-3.9427	-1.5429	0.2545
C	-4.0304	-2.7968	-0.3381
C	-2.8087	-3.4129	-0.712
C	-1.5982	-2.7922	-0.4719
C	0.9912	-1.4638	0.4269
C	2.1744	-0.718	0.2887
C	2.1319	0.6766	-0.0219
C	0.912	1.3781	-0.0633
C	3.4006	1.2707	-0.2516
C	3.4467	2.6321	-0.6183
C	2.199	3.3183	-0.8006
C	0.9894	2.7278	-0.5328
C	1.149	-2.8314	0.8156
C	2.3967	-3.3844	0.957
C	3.6001	-2.6391	0.7112
C	3.4771	-1.2709	0.3882
C	-5.3869	3.2396	1.0631
C	-6.5888	2.6362	0.7362
C	-5.3225	-3.423	-0.6077
C	-6.5391	-2.7747	-0.6066
C	4.8795	-3.2895	0.8122
C	4.6874	3.3291	-0.8298
C	5.9685	2.768	-0.715

C	6.1253	-2.6748	0.613
C	-7.8582	3.3642	0.7488
C	-8.818	2.4843	0.3815
C	-8.1353	1.2076	0.1526
N	-6.8222	1.3179	0.3494
N	-6.8449	-1.4281	-0.4241
C	-8.1918	-1.2175	-0.4448
C	-8.811	-2.5056	-0.6854
C	-7.8233	-3.4317	-0.7814
C	7.4114	-3.3414	0.6877
C	8.3635	-2.4037	0.4223
C	7.6672	-1.1504	0.1888
N	6.3381	-1.3581	0.3079
N	6.2557	1.4645	-0.4143
C	7.597	1.3094	-0.3976
C	8.2235	2.5861	-0.6929
C	7.2176	3.4831	-0.8929
C	8.2738	0.0922	-0.1271
C	-8.82	0.0024	-0.2232
C	9.7561	0.1207	-0.1824
C	4.6356	4.7743	-1.1935
C	4.913	-4.742	1.1483
C	-5.4044	4.6909	1.4095
C	-5.3187	-4.8765	-0.9395
C	-10.2961	0.0377	-0.343
C	-11.1126	0.2893	0.7637
C	-12.4995	0.3315	0.6624
C	-13.1046	0.105	-0.5713
C	-12.3202	-0.1569	-1.6911
C	-10.934	-0.1846	-1.5668
C	10.527	-0.059	0.9687
C	11.9177	-0.0345	0.9287
C	12.5655	0.1744	-0.2862
C	11.8224	0.3566	-1.4498
C	10.4326	0.3273	-1.387
C	4.5657	5.7457	-0.1784
C	4.5103	7.0933	-0.5423
C	4.5204	7.4983	-1.8802
C	4.5838	6.5107	-2.8669
C	4.6431	5.1512	-2.5485
C	4.8349	-5.6966	0.1184
C	4.8687	-7.0521	0.4562
C	4.9723	-7.4805	1.7824

C	5.0491	-6.509	2.7845
C	5.0205	-5.143	2.4923
C	-5.4145	-5.2963	-2.2787
C	-5.3796	-6.6665	-2.5599
C	-5.2555	-7.6245	-1.552
C	-5.1559	-7.1801	-0.2291
C	-5.1801	-5.8231	0.0957
C	-5.4407	5.0788	2.7621
C	-5.4282	6.44	3.074
C	-5.3745	7.4241	2.082
C	-5.3289	7.0114	0.7482
C	-5.3431	5.6593	0.3915
C	-5.2433	-9.0916	-1.8695
C	-5.0712	-5.3777	1.525
C	-5.5417	-4.2986	-3.3947
C	-5.5013	4.0442	3.8482
C	-5.3896	8.8812	2.443
C	-5.2911	5.252	-1.053
C	4.5501	5.3391	1.2667
C	4.4918	8.9541	-2.2454
C	4.7045	4.1117	-3.6301
C	5.103	-4.121	3.5891
C	4.9713	-8.9422	2.1247
C	4.7228	-5.2649	-1.3151
F	9.7507	0.495	-2.5093
F	12.4397	0.549	-2.6027
F	13.8835	0.1998	-0.3347
F	12.6254	-0.2015	2.0327
F	9.9365	-0.2518	2.1378
F	-10.5679	0.4929	1.9543
F	-10.2168	-0.4293	-2.6539
H	-4.8948	0.6527	0.9593
H	-0.7476	3.2984	1.0215
H	-2.8959	4.3988	1.3167
H	-4.8421	-1.0787	0.6361
H	-2.8265	-4.3838	-1.211
H	-0.6866	-3.2886	-0.803
H	2.2123	4.3428	-1.179
H	0.0823	3.2908	-0.7438
H	0.2768	-3.439	1.0544
H	2.4797	-4.4251	1.2776
H	-7.9755	4.4145	1.0088
H	-9.8832	2.6739	0.2637

H	-6.2271	-0.6252	-0.3338
Pd	4.8966	0.0278	0.009
H	-9.8836	-2.6768	-0.7413
H	-7.9327	-4.5035	-0.9322
H	7.5568	-4.3969	0.9084
H	9.4408	-2.5505	0.3772
H	9.2943	2.7753	-0.7315
H	7.3041	4.5407	-1.1336
F	-13.2458	0.5703	1.7283
F	-14.4202	0.1369	-0.6779
F	-12.895	-0.3687	-2.8636
H	4.4549	7.8495	0.2465
H	4.5838	6.8047	-3.9208
H	4.8136	-7.7955	-0.3447
H	5.1349	-6.8219	3.8295
H	-5.4461	-6.9923	-3.6022
H	-5.0555	-7.9136	0.5768
H	-5.4585	6.74	4.1259
H	-5.2762	7.7643	-0.0439
H	-4.4378	-9.6118	-1.3294
H	-6.191	-9.5673	-1.5679
H	-5.1086	-9.2706	-2.9453
H	-4.1647	-4.773	1.6875
H	-5.9256	-4.7451	1.8121
H	-5.0332	-6.2376	2.2073
H	-6.5301	-3.8114	-3.3893
H	-4.7948	-3.495	-3.304
H	-5.4116	-4.7827	-4.3721
H	-6.408	3.4256	3.757
H	-4.6444	3.3542	3.7928
H	-5.5018	4.5104	4.8427
H	-4.805	9.0761	3.3541
H	-4.9842	9.5022	1.6317
H	-6.4186	9.2261	2.6394
H	-4.4815	4.5288	-1.238
H	-6.2272	4.7613	-1.3634
H	-5.1306	6.122	-1.7041
H	4.4965	6.2161	1.9258
H	3.6892	4.6889	1.4889
H	5.4529	4.7659	1.5302
H	5.5135	9.3672	-2.2888
H	4.0339	9.1133	-3.2322
H	3.9341	9.5447	-1.5043

H	3.8813	3.3861	-3.5346
H	4.6438	4.5708	-4.626
H	5.6406	3.5335	-3.5763
H	6.0034	-3.4949	3.4853
H	4.2402	-3.4369	3.563
H	5.1319	-4.5998	4.5771
H	5.3614	-9.5507	1.2963
H	3.9477	-9.2944	2.3357
H	5.5757	-9.1467	3.0203
H	3.8307	-4.6388	-1.4744
H	5.5905	-4.6582	-1.619
H	4.6582	-6.1311	-1.9872