

Supplementary Materials

How computations can assist the rational design of drugs for photodynamic therapy: photosensitizing activity assessment of a Ru(II)-BODIPY assembly

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Table S1

	λ	eV	f	MO contribution ^a	$\lambda_{\text{exp}}^{\text{q}}$
B3LYP-D3	644	1.93	1.0358	H→L, 99%	641
B3PW91	642	1.93	1.0386	H→L, 100%	
camB3LYP-D3	594	2.09	1.1050	H→L, 96%	
B97D	705	1.76	0.9437	H→L, 99%	
ω B97XD	587	2.11	1.1106	H→L, 94%	
TPSS	693	1.79	0.9653	H→L, 99%	
PBE0	630	1.97	1.0632	H→L, 100%	
PBE	710	1.75	0.9289	H→L, 99%	
M06	639	1.94	1.0452	H→L, 100%	
M11	578	2.15	1.0900	H→L, 92%	
MN12L	640	1.94	1.1056	H→L, 99%	
MN15	627	2.01	1.0619	H→L, 98%	
MN15L	637	1.95		H→L, 100%	

^a data in CH₃CN from ref [1].

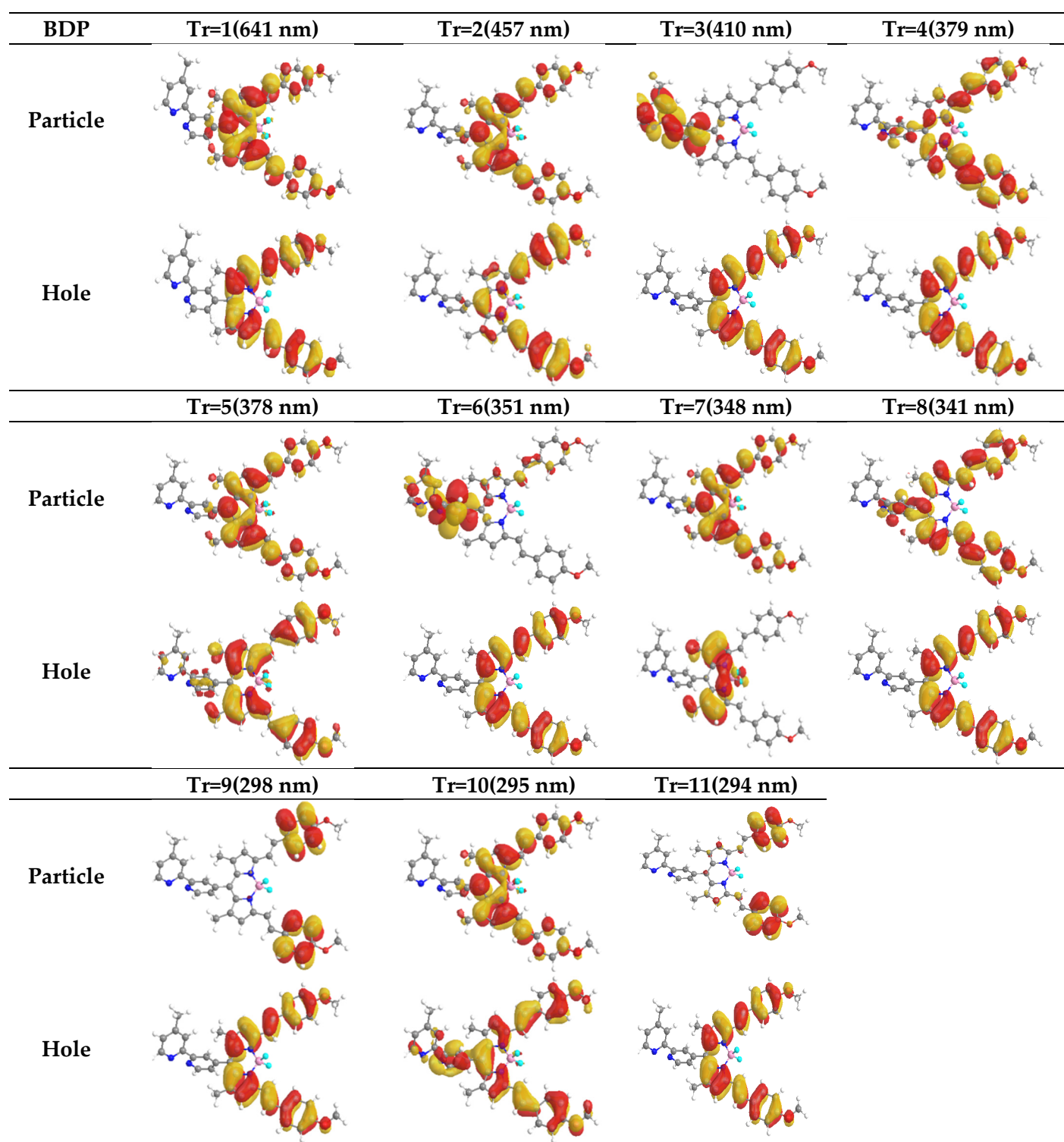


Figure S1

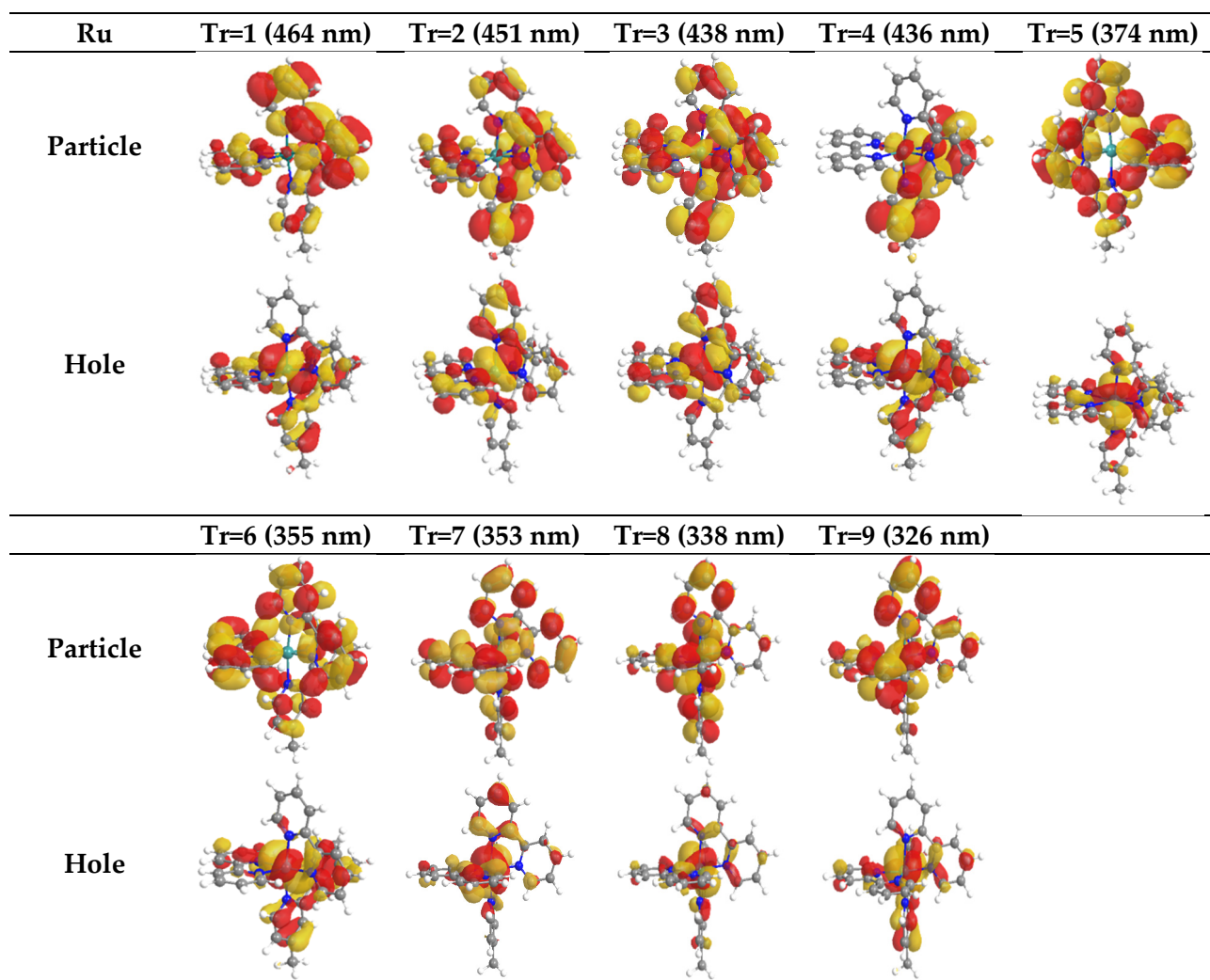


Figure S2

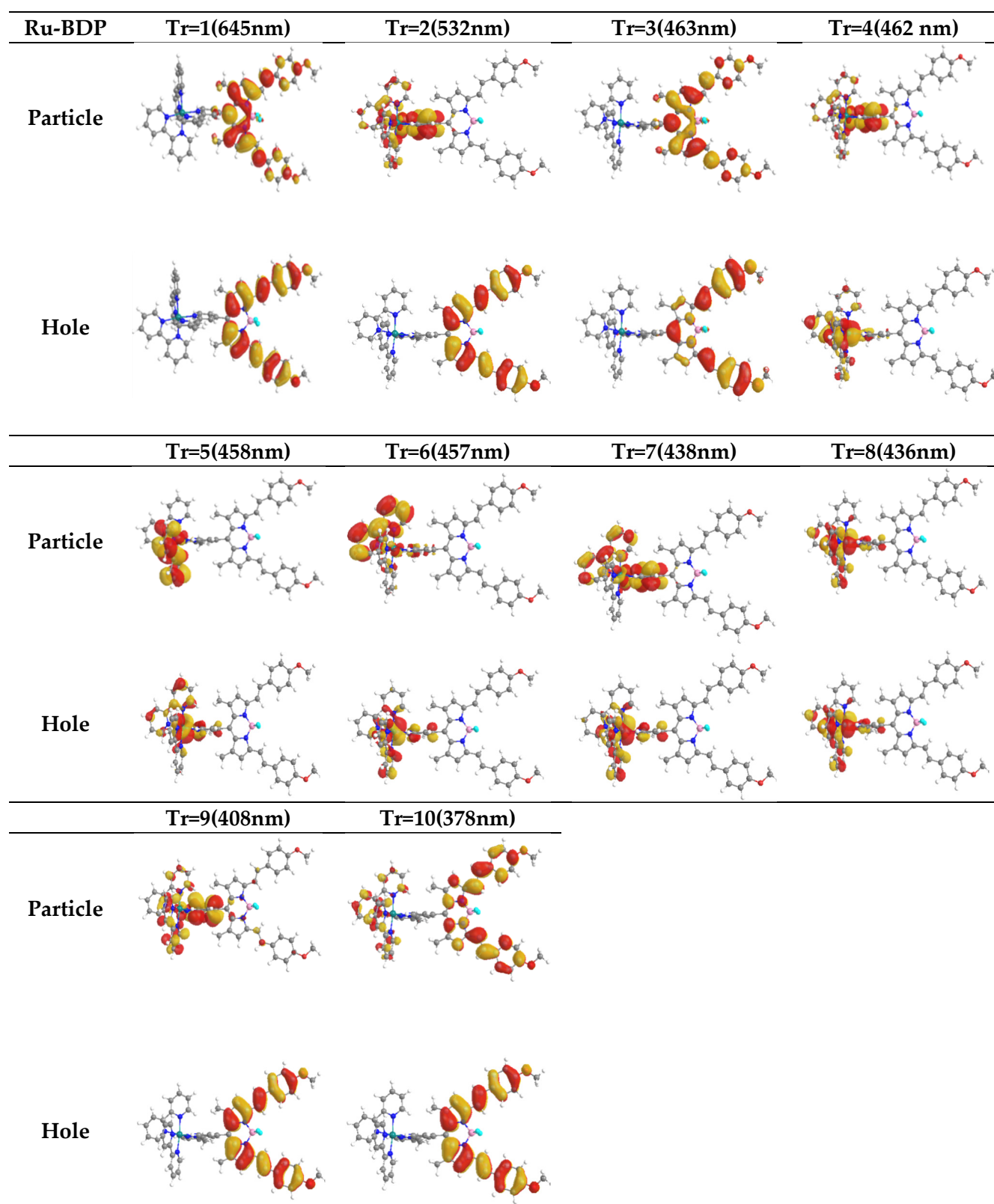


Figure S3

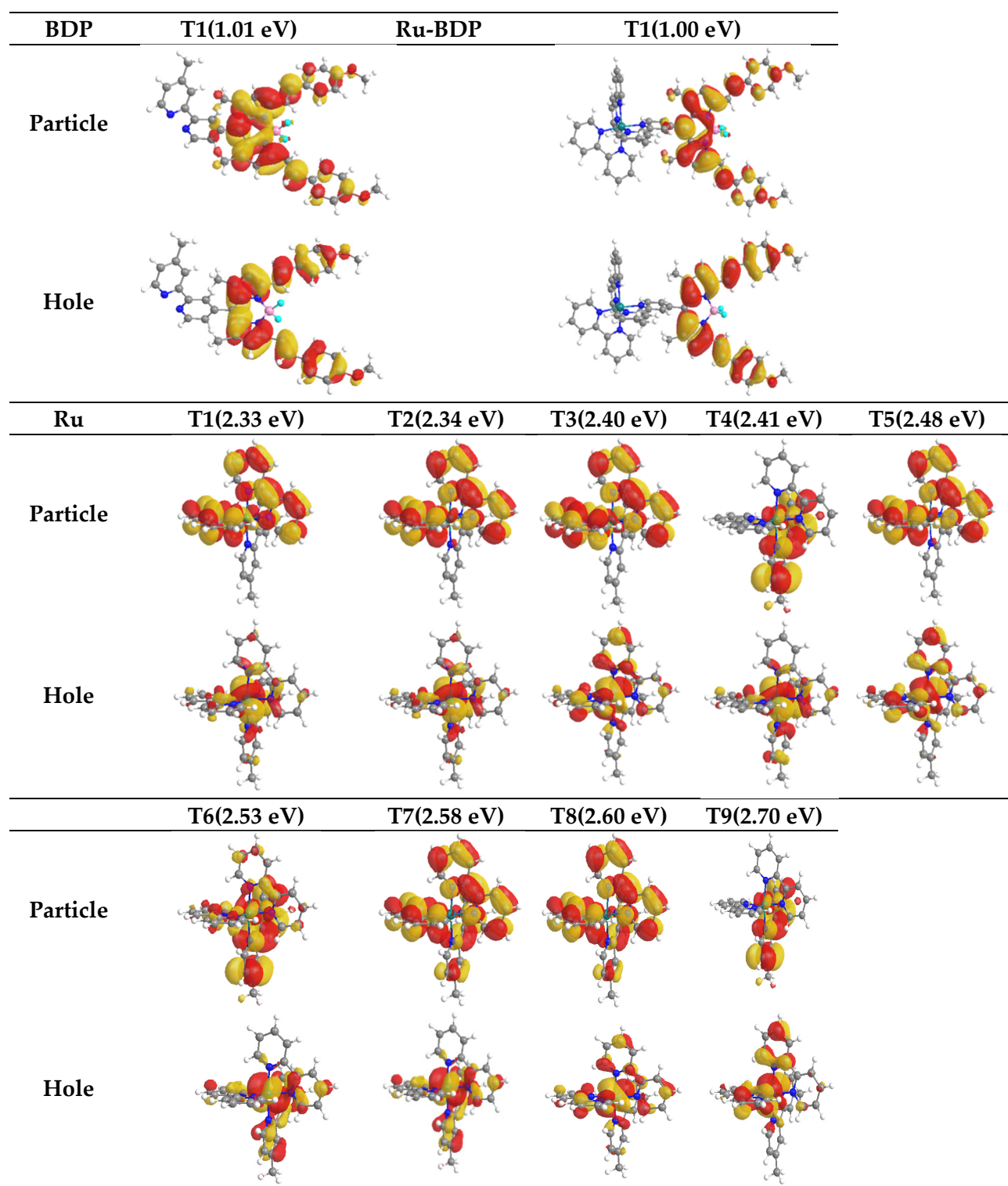


Figure S4

Table S2

Angle	E _{rel} (kcal mol ⁻¹)	λ_{max} (nm)	T1,T2 (eV)	$\Delta E_{\text{S1-Tm}}$ (eV)	SOC (cm ⁻¹)
0	21.3	883	0.54, 1.39	0.86, 0.0	1.5, 5.0
10	18.1	741	0.80	0.85	1.4
20	13.1	735	0.84	0.85	1.4
30	8.9	717	0.87	0.86	1.3
40	5.6	702	0.90	0.86	1.3
50	3.2	687	0.93	0.87	1.3
60	1.6	674	0.95	0.89	3.1
70	0.6	660	0.98	0.90	1.2
80	0.2	650	0.99	0.92	1.0
90	0.0	645	1.00	0.93	0.9

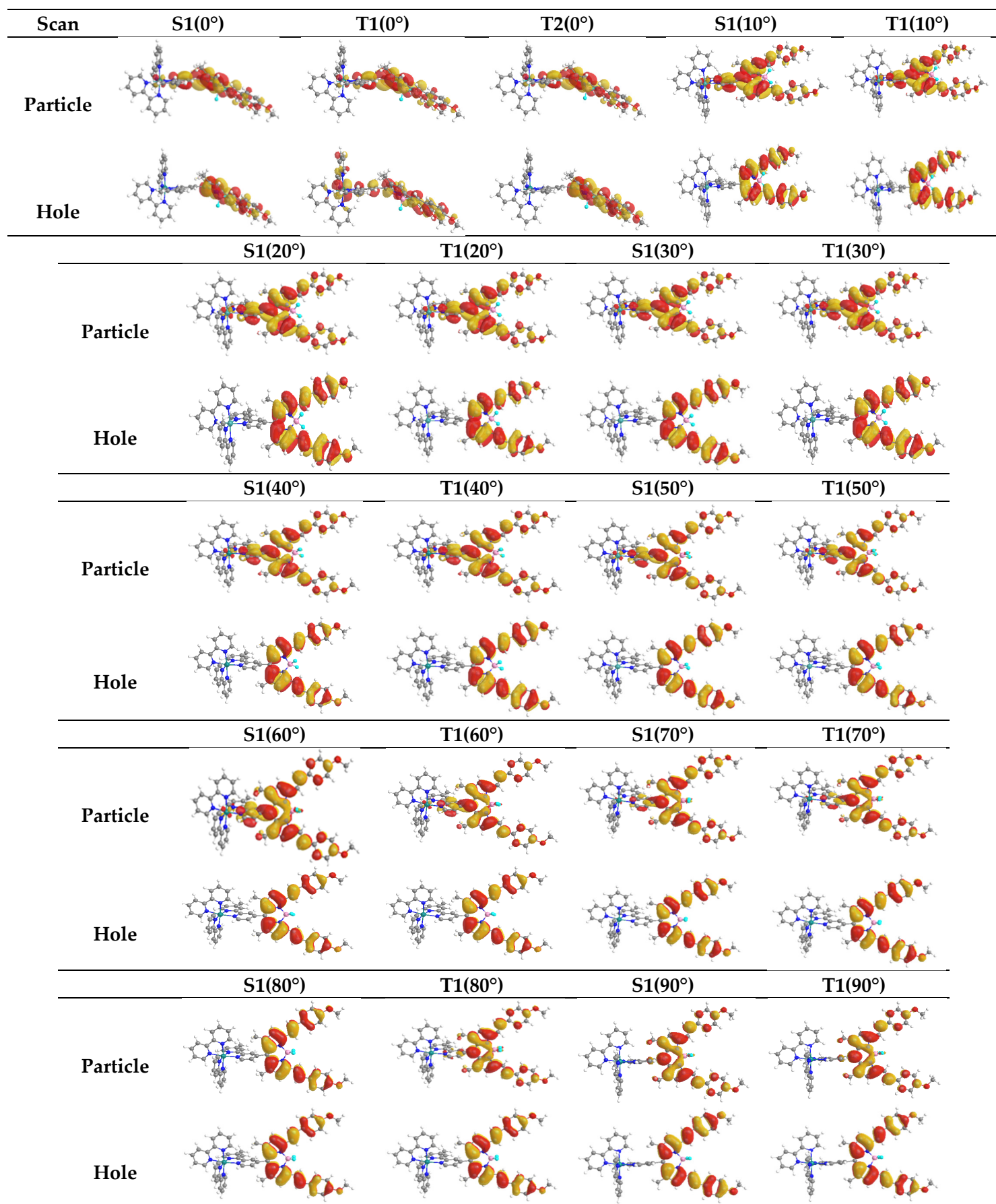


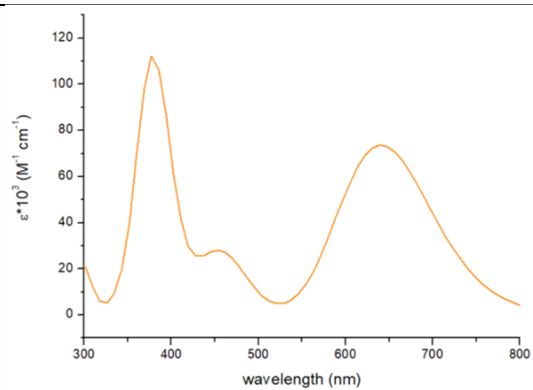
Figure S5

Table S3

Ru-HBDP

Tr ^a	Band	State	ΔE	λ	f	MO contribution	Theoretical Assignment
1	I	S1	1.81	686	0.89	H→L 100%	LMCT
2	II		2.10	591	0.05	H-1→L 92%	MLCT/ LMCT
3			2.27	545	0.45	H-2→L 96%	
4			2.45	505	0.06	H→L+1 78%	
5			2.58	481	0.36	H-4→L 89%	
6			2.60	477	0.02	H→L+3 52%, H→L+2 27%, H→L+1 20%,	
7			2.72	455	0.01	H-2→L+1 45%, H-2→L+2 16%, H-2→L+3 14%	
8			2.80	443	0.07	H-3→L+1 59%, H-2→L+2 15%	
9			2.87	431	0.08	H-3→L+3 62%, H-2→L+2 23%	
10	III		2.88	430	0.12	H-2→L+3 38%, H-3→L+2 36%	MLCT/ ILCT
11			3.11	399	0.04	H-5→L 70%	
12			3.15	393	0.09	H→L+4 71%, H- 5→L 17%,	
13			3.27	378	1.17	H→L+5 81%	
		<i>T1</i>	0.92			<i>H→L 98%</i>	<i>LMCT</i>

Ru-HBDP

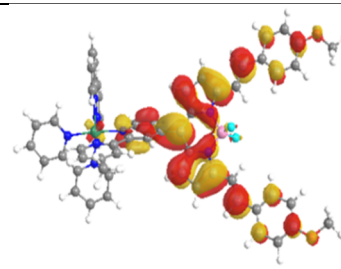
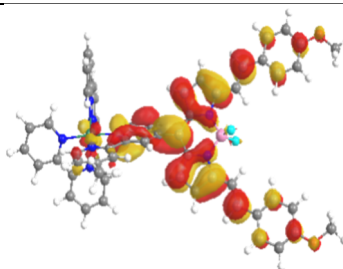
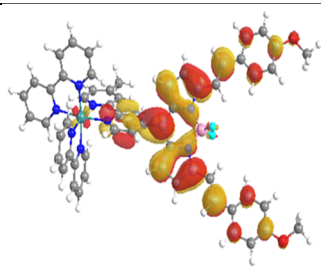


Tr=1(686 nm)

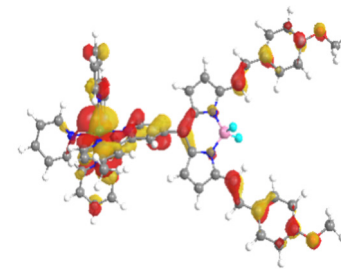
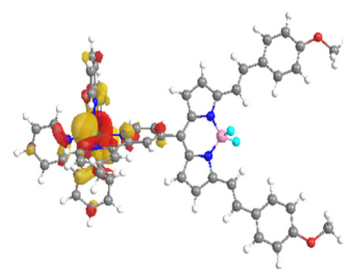
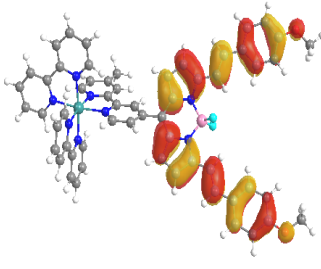
Tr=2(591 nm)

Tr=3(545nm)

Particle



Hole

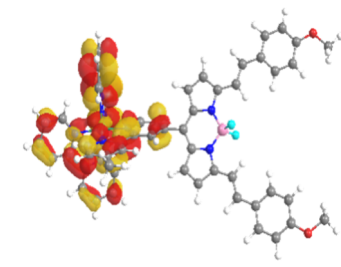
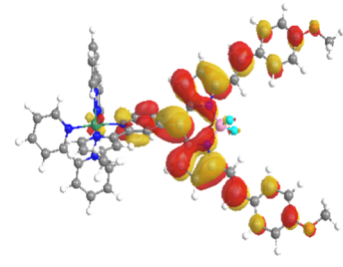
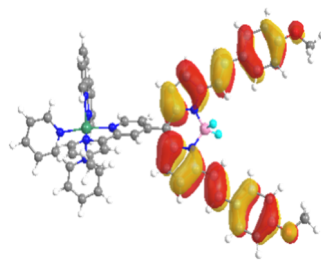


Tr=4(505 nm)

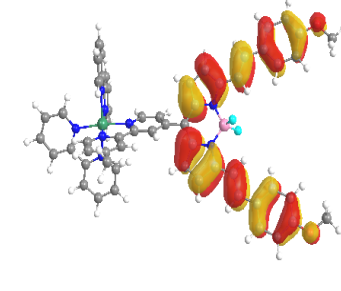
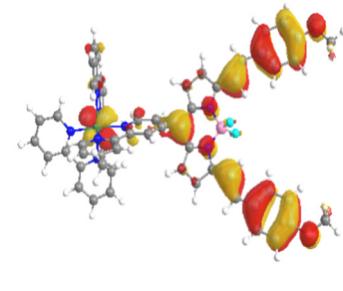
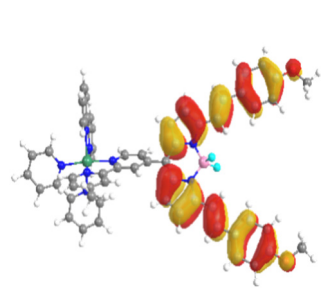
Tr=5(481 nm)

Tr=6(477 nm)

Particle



Hole



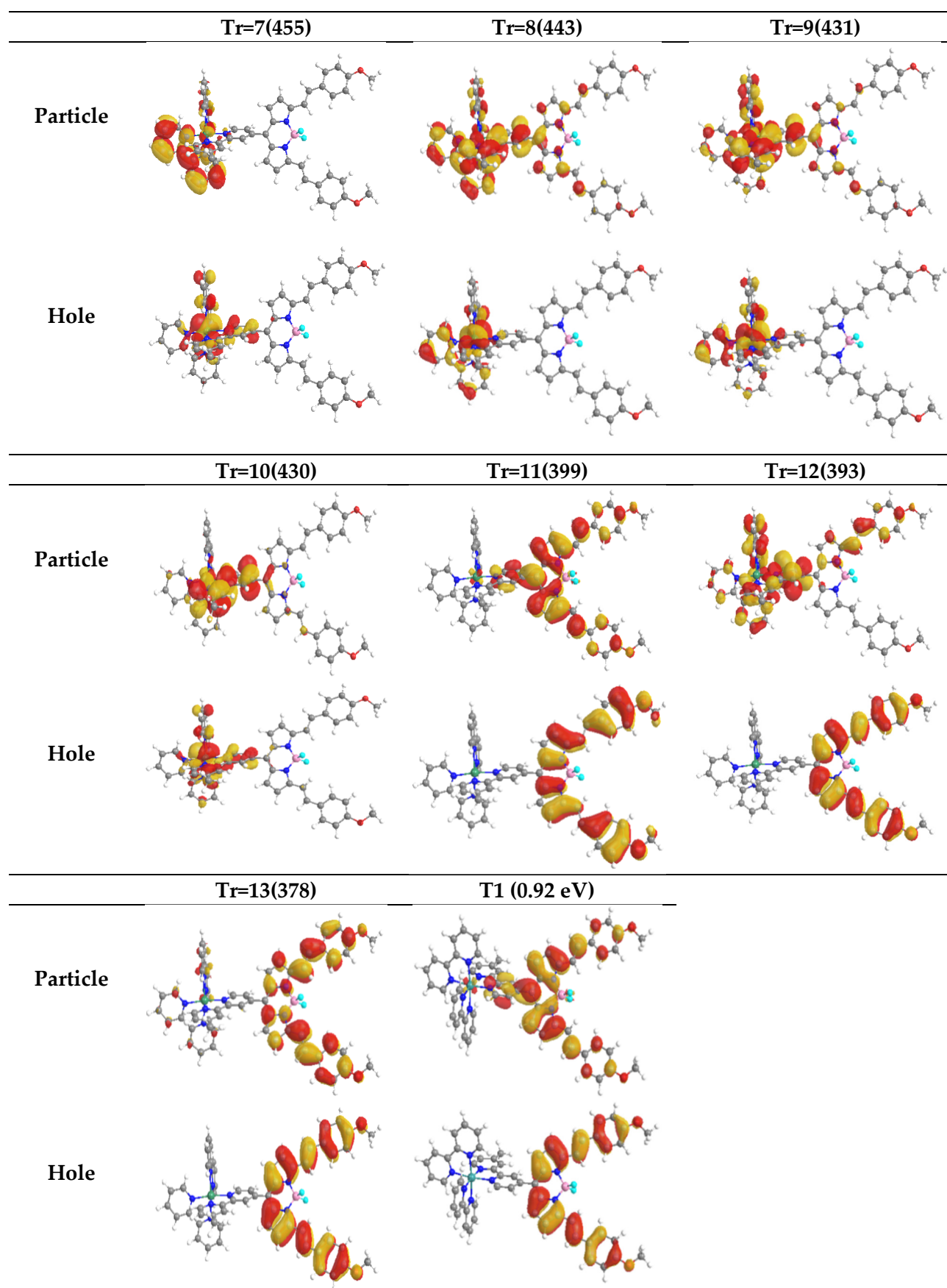


Figure S6

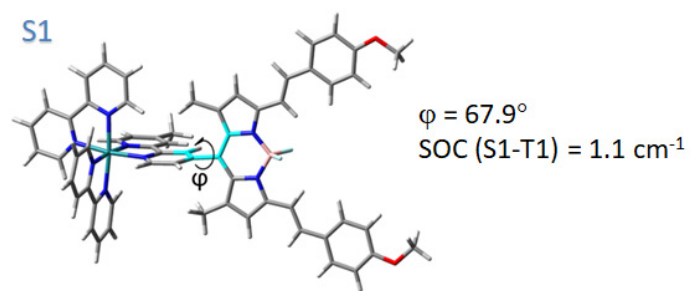


Figure S7

References

1. Qiao, L.; Liu, J.; Han, Y.; Wei, F.; Liao, X.; Zhang, C.; Xie, L.; Ji, L.; Chao, H. Rational Design of a Lysosome-Targeting and near-Infrared Absorbing Ru(II)–BODIPY Conjugate for Photodynamic Therapy. *Chem. Commun.* **2021**, 57, 1790–1793.