Supporting Information

for

Anionic Ancillary Ligands in Cyclometalated Ru(II) Complexes Sensitizers Improves the Photovoltaic Efficiency of Dye-sensitized Solar Cells：Insights from Theoretical Investigations

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Figure S1 Calculated absorption spectra for dyes BTP using different function dissolved in DMF solution.

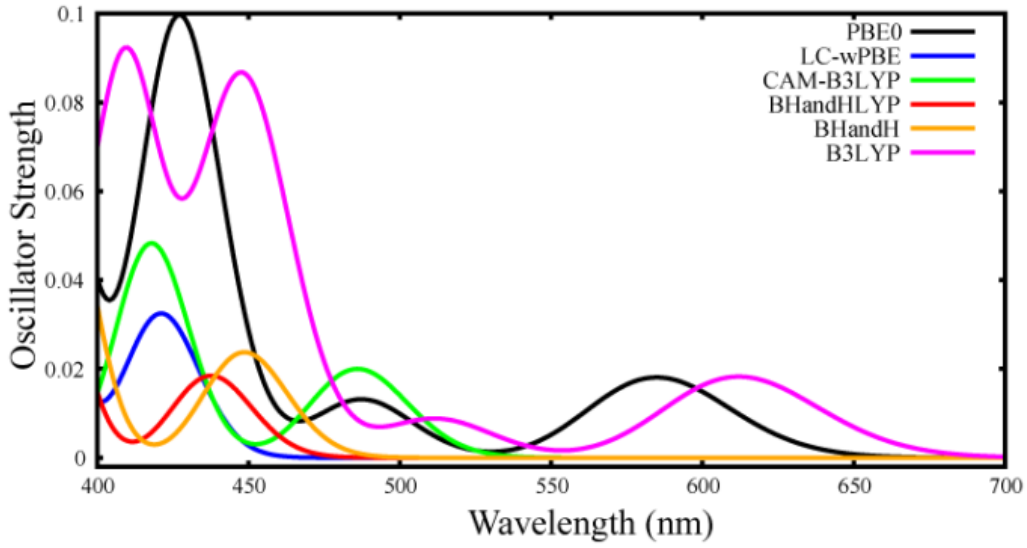

Figure S2. The optimized geometries of adsorption systems.

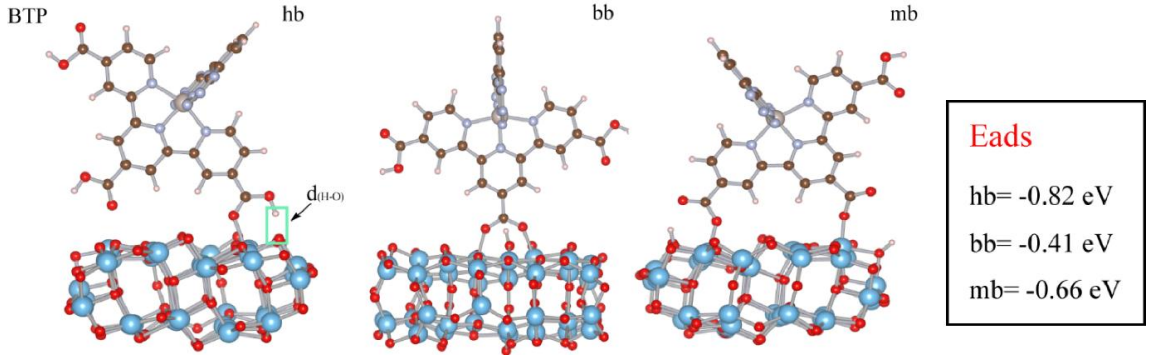

Table S1 The optimized main geometry parameters for BTP, BATP and BMTP in ground state, at B3LYP/LanL2DZ level of theory, in comparison with available experimental value of BMTP (Bond in Å ; Angle in deg.)

	BPT	BATP	BMTP ^{Expt}	BMTP
Ru N19	1.97	2.00	1.96	2.016
Ru1 N1	2.08	2.07	2.03	2.070
Ru1 N7	2.10	2.06	2.05	2.126
Ru1 N13	2.10	2.14	2.06	2.095
Ru1 N25	2.09	2.11	2.07	2.131
Ru1 N31	2.09	2.11	2.07	2.132
N19 Ru1 N1	179.80	178.76	176.55	178.38
N19 Ru1 N7	103.20	100.80	102.68	104.19
N1 Ru1 N7	76.79	77.96	78.35	77.41
N19 Ru1 N13	103.20	105.23	101.37	101.49
N1 Ru1 N13	76.79	75.99	77.56	76.88
N7 Ru1 N13	153.58	153.96	155.92	154.30
N19 Ru1 N25	79.10	78.67	79.58	78.33
N1 Ru1 N25	101.08	101.32	97.14	101.71
N7 Ru1 N25	92.48	91.16	91.52	92.83
N13 Ru1 N25	92.48	93.86	91.54	92.24
N19 Ru1 N31	79.18	78.77	79.48	78.54
N1 Ru1 N31	100.62	101.17	103.83	101.39
N7 Ru1 N31	92.44	91.05	91.62	92.69
N13 Ru1 N31	92.44	93.98	94.01	92.42
N25 Ru1 N31	158.29	157.35	159.00	156.88