

Supporting information

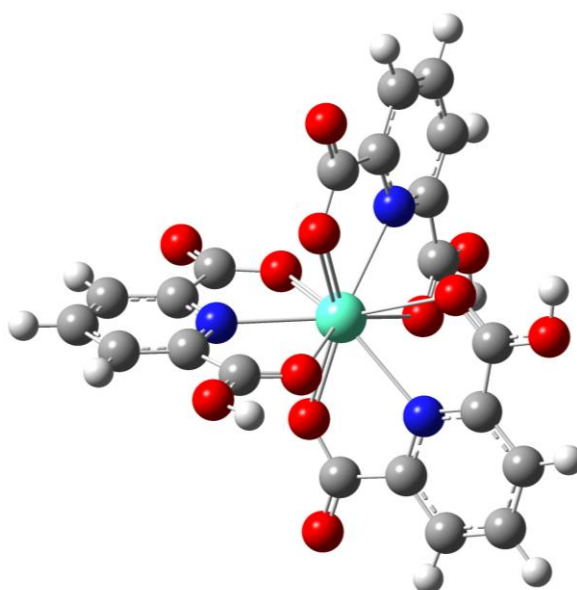
Table S1. Selected Bond Distances (Å) for Complexes 1–2

	Tb1	Dy1
Ln(1)–O(5)#1	2.422(4)	2.543(7)
Ln(1)–O(5)	2.422(4)	2.498(5)
Ln(1)–O(3)#1	2.425(5)	2.487(7)
Ln(1)–O(3)	2.425(5)	2.343(7)
Ln(1)–O(1)#1	2.447(5)	2.334(7)
Ln(1)–O(1)	2.447(5)	2.331(5)
Ln(1)–N(2)	2.513(7)	2.476(9)
Ln(1)–N(1)	2.515(5)	2.495(5)
Ln(1)–N(1) #1	2.515(5)	2.525(9)

^aSymmetry transformations used to generate equivalent atoms: #1 -x,y,-z+1/2

Table S2 Selected angles [°] for Complexes 1–2

Ln=Tb, Dy	Tb1	Dy1
O(7)- Ln(1)-O(5)	127.7(2)	128.2(14)
O(7)- Ln(1)-O(11)	78.05(16)	80.8(2)
O(5)- Ln(1)-O(11)	147.81(16)	143(4)
O(5)- Ln(1)-O(1)	87.1(3)	89.2(3)
O(7)- Ln(1)-N(2)	63.83(10)	65.7(3)
O(11)- Ln(1)-N(2)	136.44(13)	141.2(2)
O(9)- Ln(1)-N(2)	73.46(16)	75.06(18)
N(3)- Ln(1)-N(1)	120.2(2)	120.7(3)



(a) Molecular structure of **Tb1**

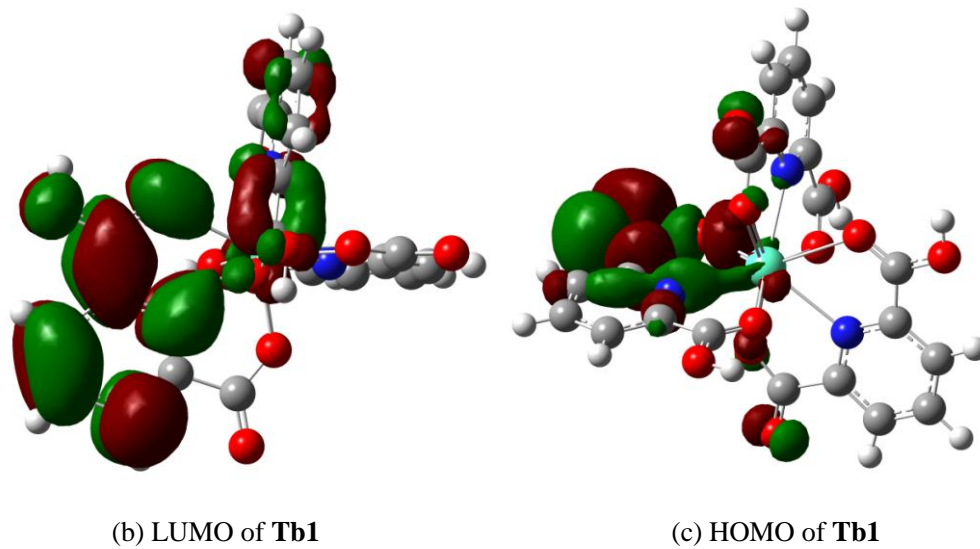
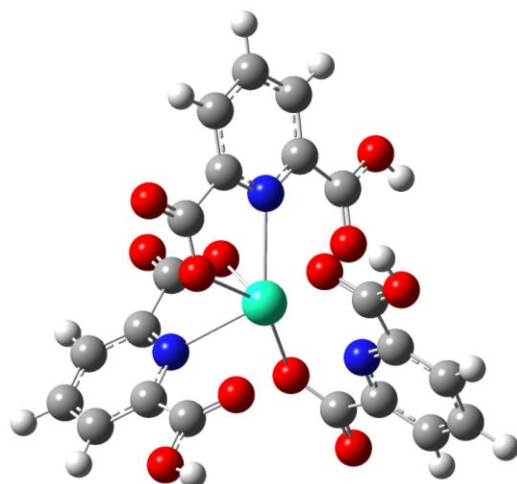
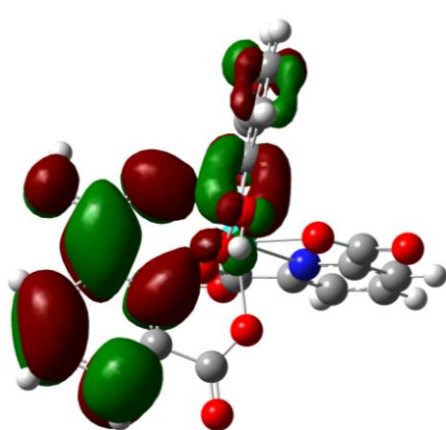


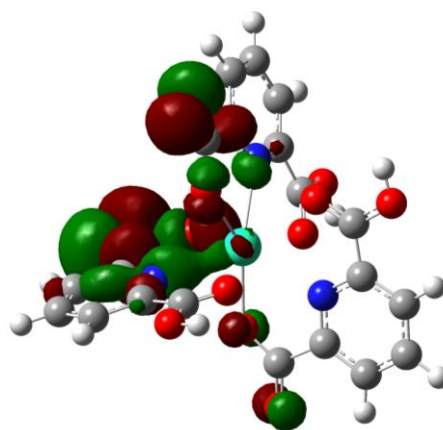
Figure S1. The structures and frontier molecular orbitals (FMOs) of **Tb1** with f orbitals



(a) Molecular structure of **Dy1**



(b) LUMO of **Dy1**



(c) HOMO of **Dy1**

Figure S2. The structures and frontier molecular orbitals (FMOs) of **Dy1** with *f* orbitals.

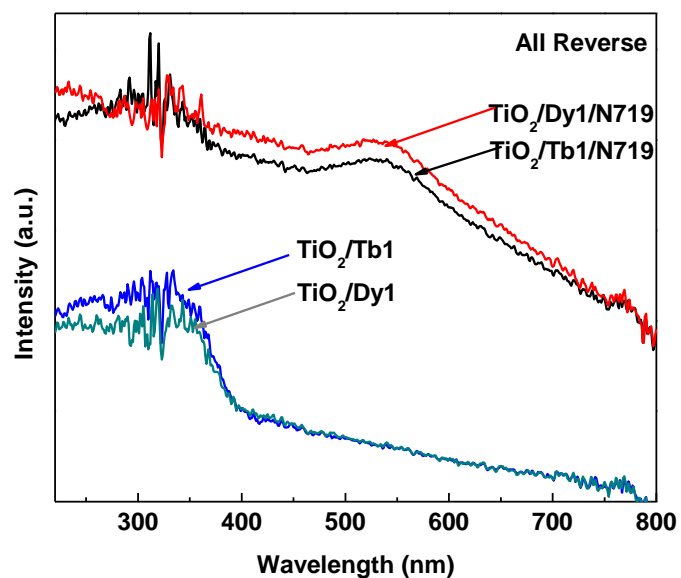


Figure S4 . SPS of lanthanide complex co-sensitized TiO_2 and raw TiO_2 .

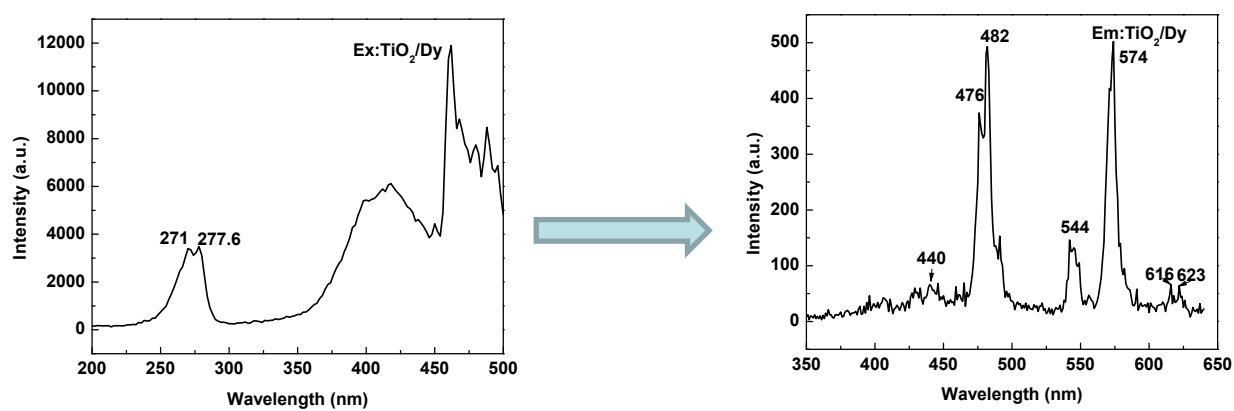


Figure S5. Solid-state emission spectrum for Dy1 (excited at 270 nm) at room temperature.

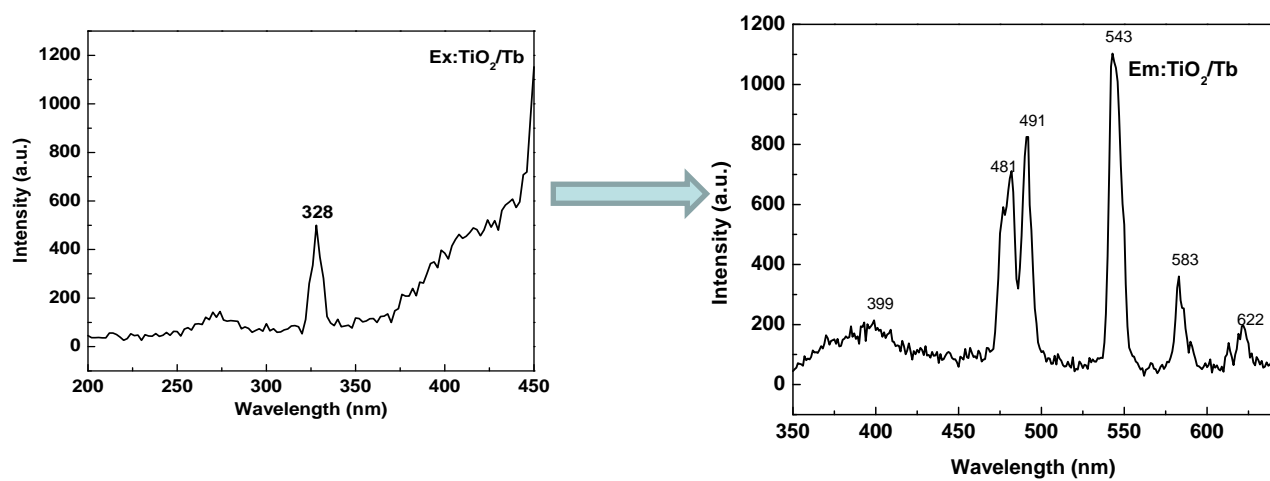


Figure S6. Solid-state emission spectrum for Tb1 (excited at 328 nm) at room temperature.