

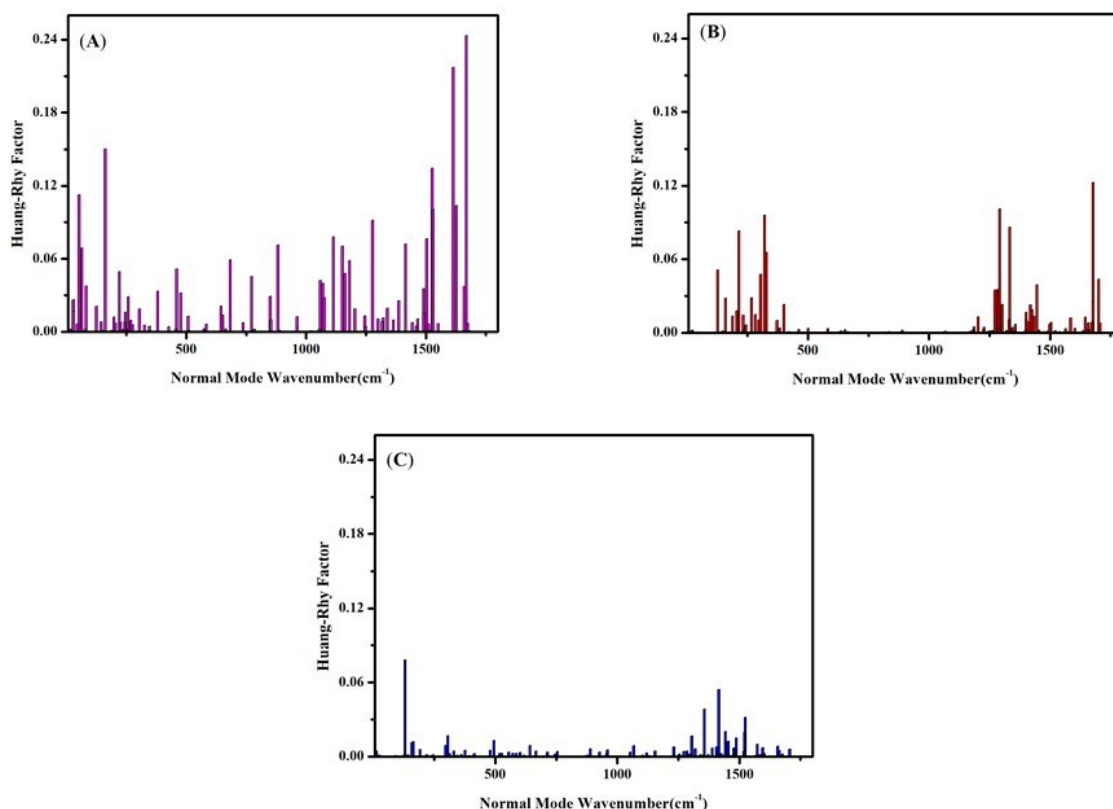
Computational studies on the materials combining graphene quantum dots and tridentate Au(III) Complexes

Support materials

Table S1: Important structural parameters based on different functional calculations

	B3LYP	PBE0	PBE0 (CH ₂ Cl ₂)	exp ¹
Au-N(1)	2.078	2.058	2.050	2.035
Au-C(1)	2.088	2.064	2.063	2.057
Au-C(2)	2.112	2.087	2.089	2.083
Au-C(3)	2.034	2.014	2.015	2.009
C(1)-Au-N(1)	80.3	80.6	80.7	81.0
C(2)-Au-N(1)	79.2	79.6	79.7	79.9
C(1)-Au-C(3)-C(4)	89.5	107.1	88.5	88.6

Figure



calculated Huang-Rhys factors versus the normal mode wavenumber at the ground state for **Au1(A)**, **Au2(B)** and **Au3(C)**

- (1) Tang, M. C.; Lee, C. H.; Lai, S. L.; Ng, M.; Chan, M. Y.; & Yam, V. W. Versatile Design Strategy for Highly Luminescent Vacuum-Evaporable and Solution-Processable Tridentate Gold(III) Complexes with Monoaryl Auxiliary Ligands and Their Applications for Phosphorescent Organic Light Emitting Devices. *Journal of the American Chemical Society* **2017**, 139, 9341-9349.

Table S2 Critical geometric structural parameters of Au1, Au2 and Au3 ³MC state at

PBE0/LANL2DZ level

Structural parameters	Au1		Au2		Au3	
	³ MC	MECP	³ MC	MECP	³ MC	MECP
Au-N(1)	2.256	2.292	2.269	2.345	2.270	2.463
Au-C(1)	2.325	2.793	2.866	2.993	2.853	3.008
Au-C(2)	2.180	2.148	2.157	2.136	2.157	2.106
Au-C(3)	2.042	2.027	2.026	2.025	2.026	2.037
C(1)-Au-N(1)	71.78	66.29	66.28	63.58	66.33	62.23
C(2)-Au-N(1)	73.21	74.33	75.17	74.20	75.02	72.62
C(1)-Au-C(3)-C(4)	111.64	114.96	64.54	64.27	64.39	61.15

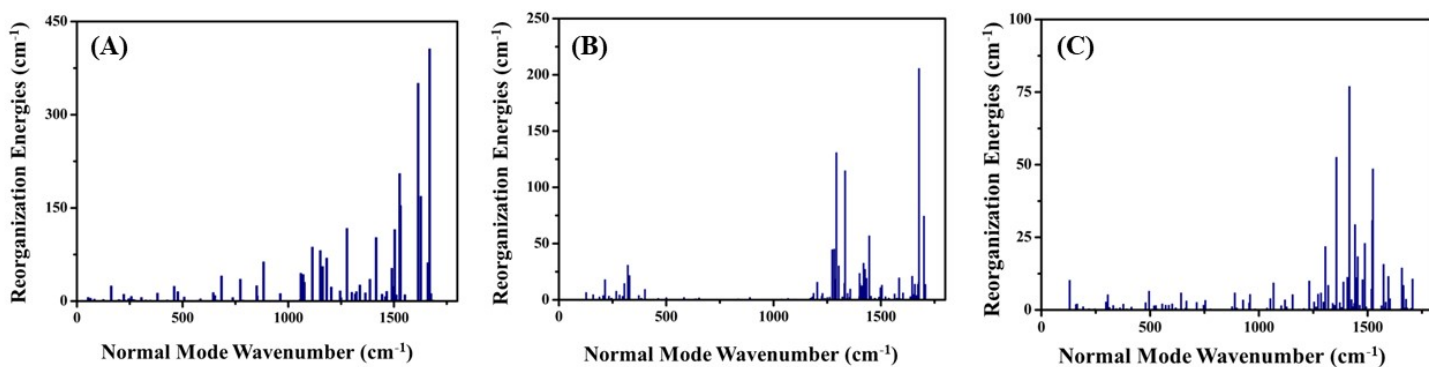


Figure S2. Reorganization energy of complexes **Au1** (A), **Au2** (B) and **Au3** (C) at regularized mode frequencies.

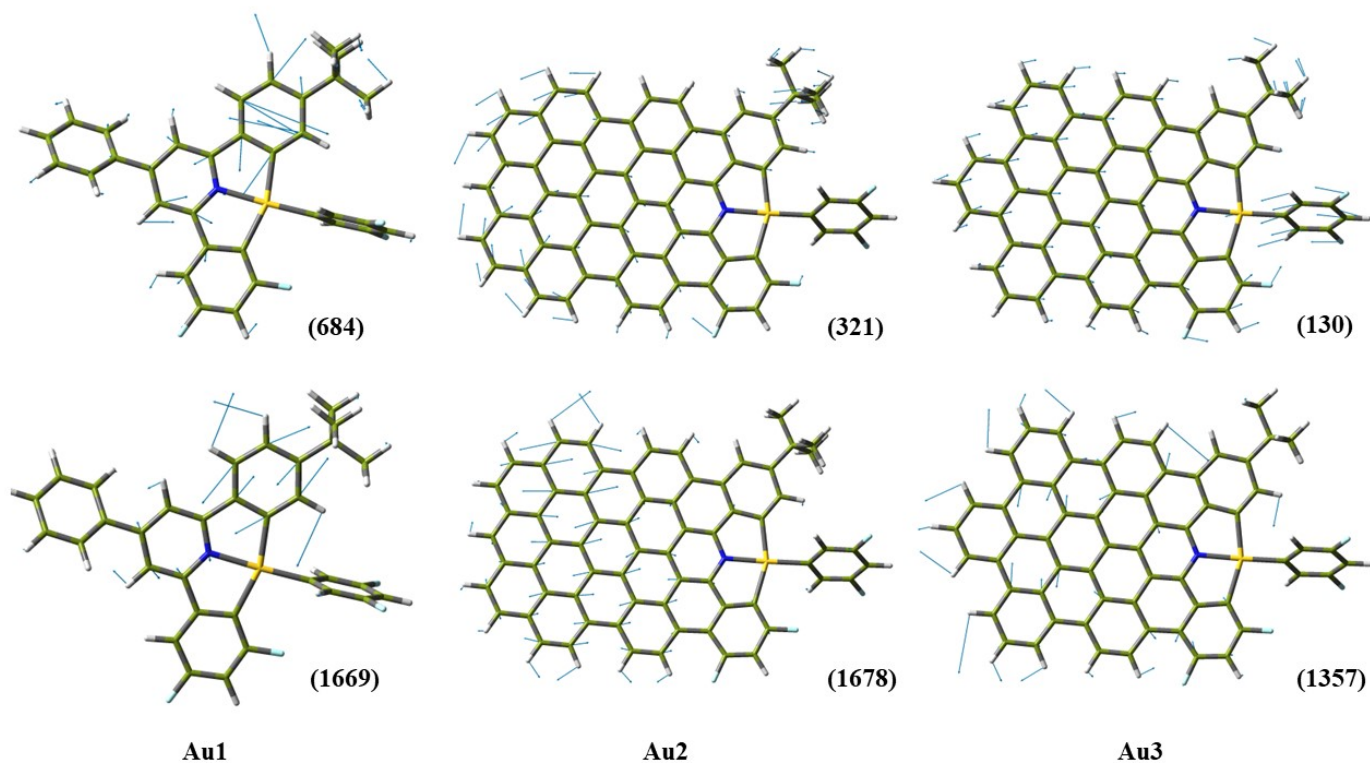


Figure S3. Positive mode displacement vectors with maximum reorganization energy and regularized mode frequencies for Au1, Au2 and Au3.

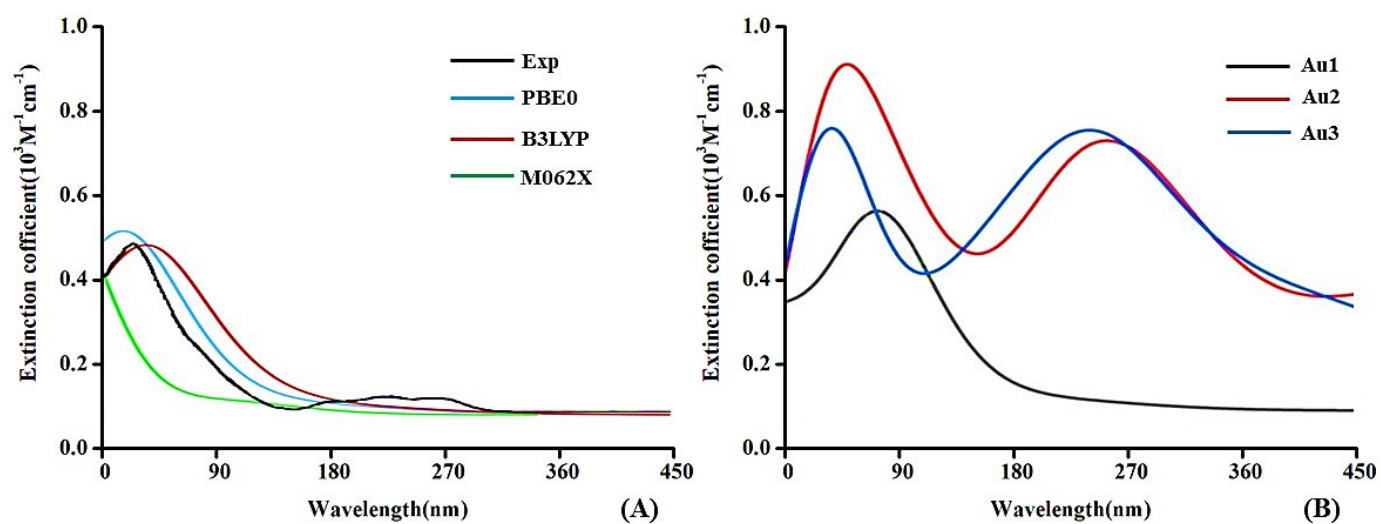


Figure S4. (A) The absorption data of Au1 based on different functional calculations and the corresponding experimental values; (B) Computational simulation of the absorption spectra of the studied complexes.