Electronic Supplementary Information (ESI)

Doping-mediated excited states dynamics of diphosphine-protected $M@Au_{12}$ (M = Au, Ir) superatoms nanocluster

Wei Pei,[*a] Lei Hou,[a] Jing Yang,[a] Si Zhou[*b,c, and] Jijun Zhao[*b,c]

[a] College of Physics Science and Technology, Yangzhou University, Yangzhou 225009, China

[b] Guangdong Basic Research Center of Excellence for Structure and Fundamental Interactions of Matter, Guangdong Provincial Key Laboratory of Quantum Engineering and Quantum Materials, School of Physics, South China Normal University, Guangzhou 510006, China

[c] Guangdong-Hong Kong Joint Laboratory of Quantum Matter, Frontier Research Institute for Physics, South China Normal University, Guangzhou 510006, China

E-mail: pwei@yzu.edu.cn, sizhou@m.scnu.edu.cn, zhaojj@dlut.edu.cn

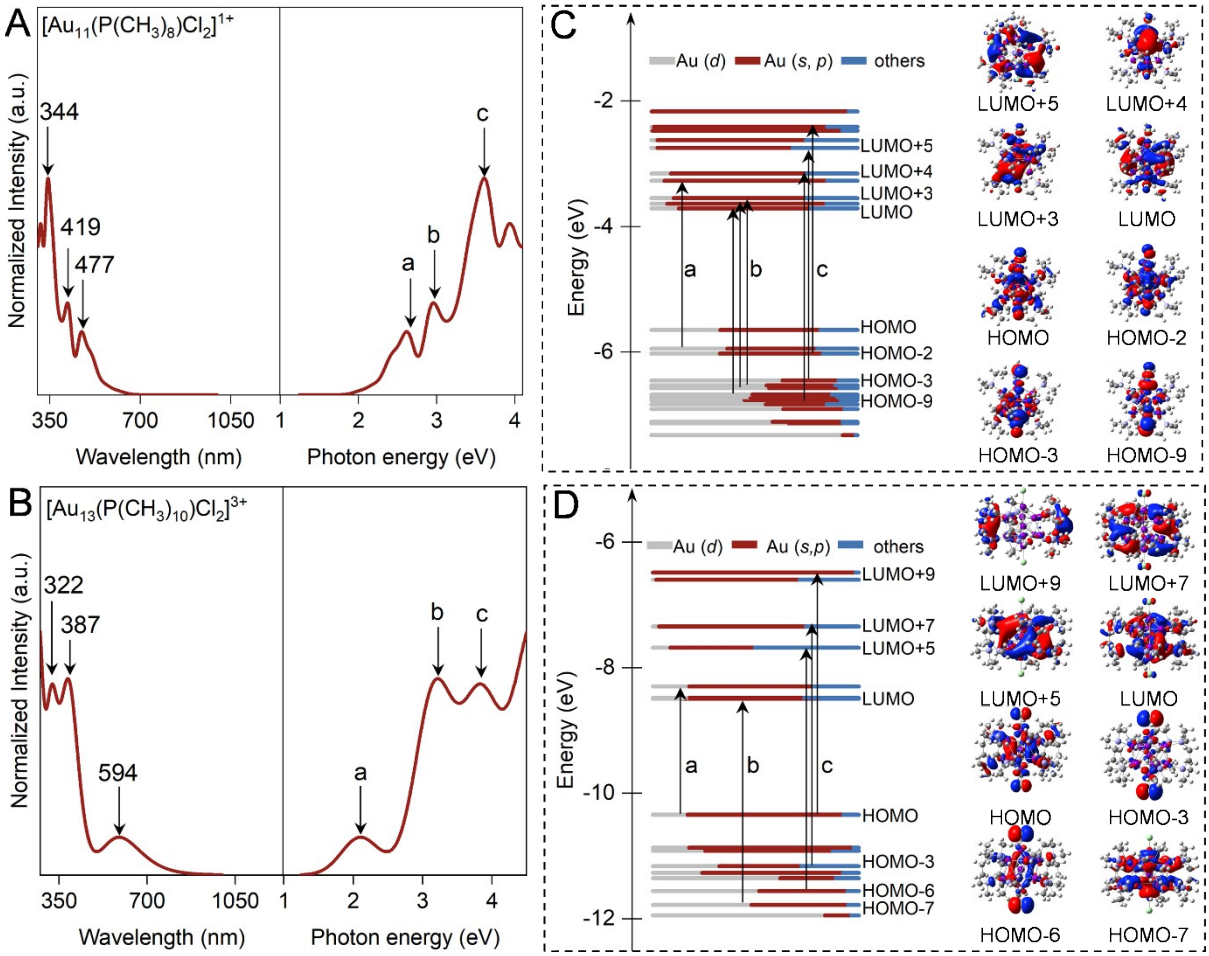

Fig. S1 (A, B) The optical absorption spectra and (C, D) the components of the Kohn–Sham molecular orbital of $[Au_{11}(PPh_3)_8Cl_2]^{1+}$ and $[Au_{13}(dppe)_5Cl_2]^{3+}$. The alphabets and numbers are the first three excited states. Red and blue colors denote positive and negative phases of the wavefunction for selected molecular orbital, respectively. The isosurface value is ± 0.02 a.u.

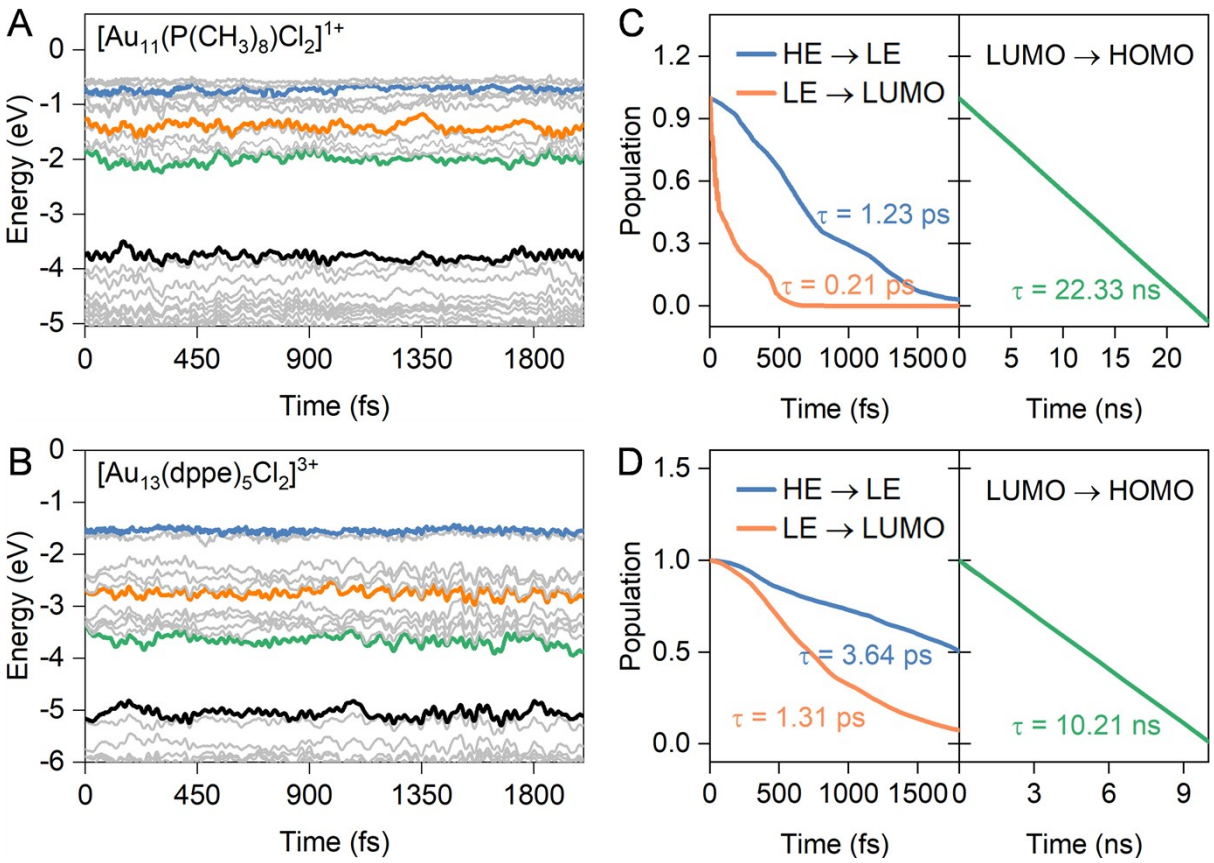

Fig. S2 Time evolution of Kohn–Sham molecular orbital of (A) $[Au_{11}(PPh_3)_8Cl_2]^{1+}$ and (B) $[Au_{13}(dppe)_5Cl_2]^{3+}$ NCs. The colored solid lines represent the high energy excited states (HE, blue), low energy excited states (LE, orange), and the lowest unoccupied molecule orbital (LUMO, green) and highest occupied molecular orbital (HOMO, black) for each ligand Au NCs, respectively. Population evolution of the initial states of the (C) $[Au_{11}(PPh_3)_8Cl_2]^{1+}$ and (D) $[Au_{13}(dppe)_5Cl_2]^{3+}$ NCs during the hot-electron relaxation process, corresponding to their lifetimes indicated by colored Arabic numerals.