Electronic Supplementary Information of

"Multiple Hybridized Resonances of IR-806 Chromonic Molecules Strongly Coupled to Au Nanorods"

Ya-Fang Zhang,^{a,‡} Da-Jie Yang,^{a,b,‡} Jia-Hong Wang,^{a,‡} Ya-Lan Wang,^a Si-Jing Ding,^a Li Zhou,^{a,*} Zhong-Hua Hao^{a,*} and Qu-Quan Wang^{a,b,*}

^{*a*} Key Laboratory of Artificial Micro- and Nano-structures of the Ministry of Education, and School of Physics and Technology, Wuhan University, Wuhan, 430072, P. R. China;

^b The Institute for Advanced Study, Wuhan University, Wuhan 430072, P. R. China.

Electronic mail: qqwang@whu.edu.cn; zhouli@whu.edu.cn; zhhao@whu.edu.cn



1. Influence of PAH on the extinction spectrum of AuNRs

Figure S1. Normalized extinction spectra of AuNRs samples (black dashed lines) and the corresponding PAH-coated ones (blue solid lines).

2. The origin of hybrid peaks around 840 and 912 nm

Poly(sodium 4-styrenesulfonate) (PSS, $M_W \approx 70,000 \text{ g/mol}$) is anionic polyelectrolyte which is usually used to assemble AuNRs and dye molecules. When IR-806 with different concentrations was dissolved in the PSS solution (dissolved in 10 mM/L NaCl aqueous solution), the extinction spectra of IR-806 red shift a little comparing with the case of aqueous solution (Figure S2(a) and (b)). However, when IR-806 was dissolved in the PAH solution, the peak around 720 nm increases and the peaks at approximately 840 and 912 nm appear (Figure S2(c)). When IR-806 molecules are adsorbed onto the PAH-coated AuNRs, the result is similar while the peak at approximately 912 nm becomes obvious (Figure S2(d)). So we can conclude that assembly processes of IR-806 induced by PAH might happen and this produces the new assembly forms of IR-806 which is the origin of these two new peaks.



Figure S2. (a) Extinction spectra of IR-806 aqueous solutions with different concentrations. Extinction spectra of IR-806 with different concentrations dissolved in the 10 mg/mL (b) PSS solution and (c) PAH solution. (d) Extinction spectra of PAH-coated AuNRs interacting with IR-806 with different concentrations. The black line represents the PAH-coated AuNRs sample.

3. Dye concentration-dependent hybridized resonances of AuNR@IR-806 nanocomplex with LSPR at 905 nm



Figure S3. (a) Extinction spectra of bare AuNRs with LSPR at 905 nm (dashed line) and corresponding AuNR@IR-806 hybrids with various dye concentrations (solid lines). The dye concentrations are 0, 0.3, 0.6, 0.8, 2.0, 5.0, and 7.0 μ M from bottom to top, respectively. The peaks are obtained by fitting their extinction spectra with Gaussian peaks. (b) The Gaussian peaks positions of the hybrids versus the dye concentration.

4. Dye concentration-dependent hybridized resonances of AuNR@IR-806 nanocomplex with LSPR at 727 nm



Figure S4. (a) Extinction spectra of bare AuNRs with LSPR at 727 nm (dashed line) and corresponding AuNR@IR-806 hybrids with various dye concentrations (solid lines). The dye concentrations are 0, 0.1, 0.6, 1.0, 1.8, 3.0, and 7.0 μ M from bottom to top, respectively. The peaks are obtained by fitting their extinction spectra with Gaussian peaks. (b) The Gaussian peaks positions of the hybrids versus the dye concentration.