

## Supporting Information

### Revealing the Correlation between Size, Structure, and Fluorescence Enhancement in Ag@Au Nanocube Clusters: A High-Content Platform Approach

Jiahao Pan,<sup>a</sup> Yuchen Zhang,<sup>a</sup> Zhentao Pang,<sup>a</sup> Yu Deng,<sup>a</sup> Zhenda Lu<sup>a,b,\*</sup>

<sup>a</sup>College of Engineering and Applied Sciences, Jiangsu Key Laboratory of Artificial Functional Materials, Nanjing University, Nanjing 210093, China

<sup>b</sup>State Key Laboratory of Analytical Chemistry for Life Science, Nanjing University, Nanjing 210093, China

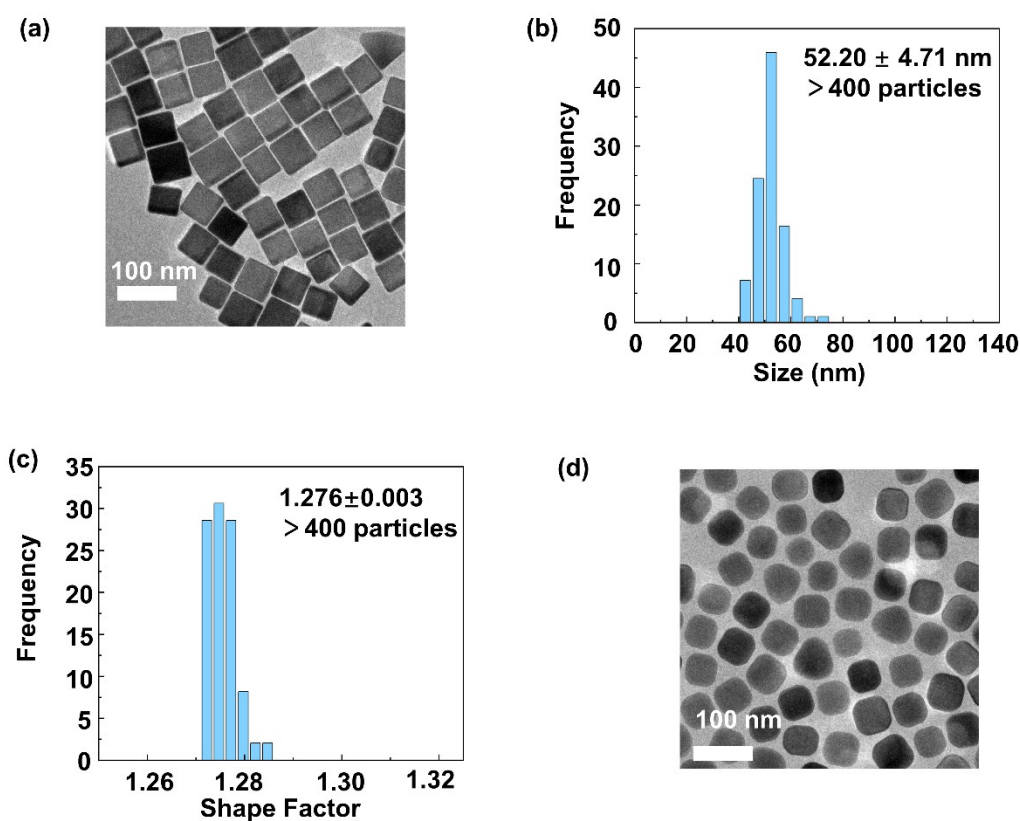
\*email: luzhenda@nju.edu.cn

### Calculation of the shape Factor

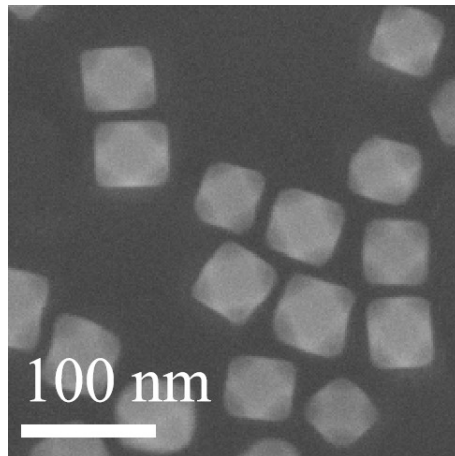
Shape characterization provides an accurate characterization of particle shape independently of particle size. Therefore, we employed the Zambelli's method to compute the shape factors of Ag nanocubes and Ag@Au nanocubes. For each particle, the so-called shape factor  $F_j$  has been computed as

$$F_j = \frac{P_j^2}{2\pi A_j}$$

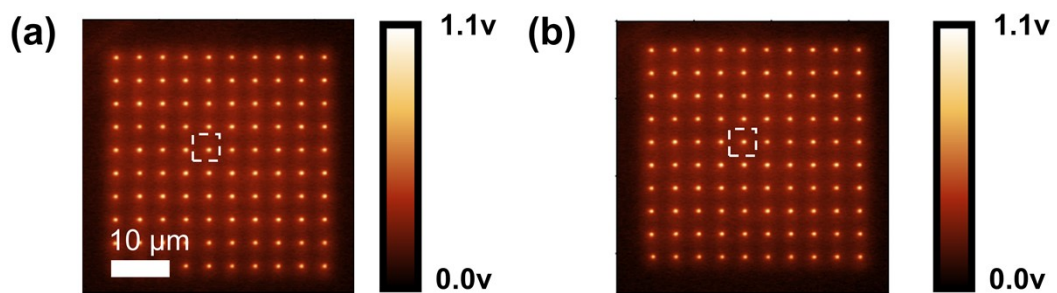
where  $P_j$  and  $A_j$  represent perimeter and area of the particle cross section.



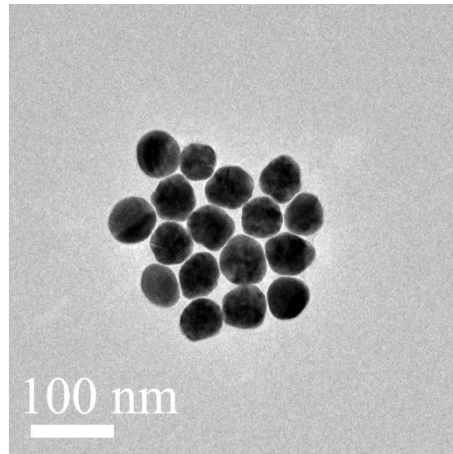
**Figure S1.** (a) TEM image of the synthesized Ag nanocubes. (b-c) The histogram of the size and shape factor frequency distribution of the Ag NCs. (d) TEM image of the Ag nanocubes before adding  $\text{HAuCl}_4$  at  $144^\circ\text{C}$ .



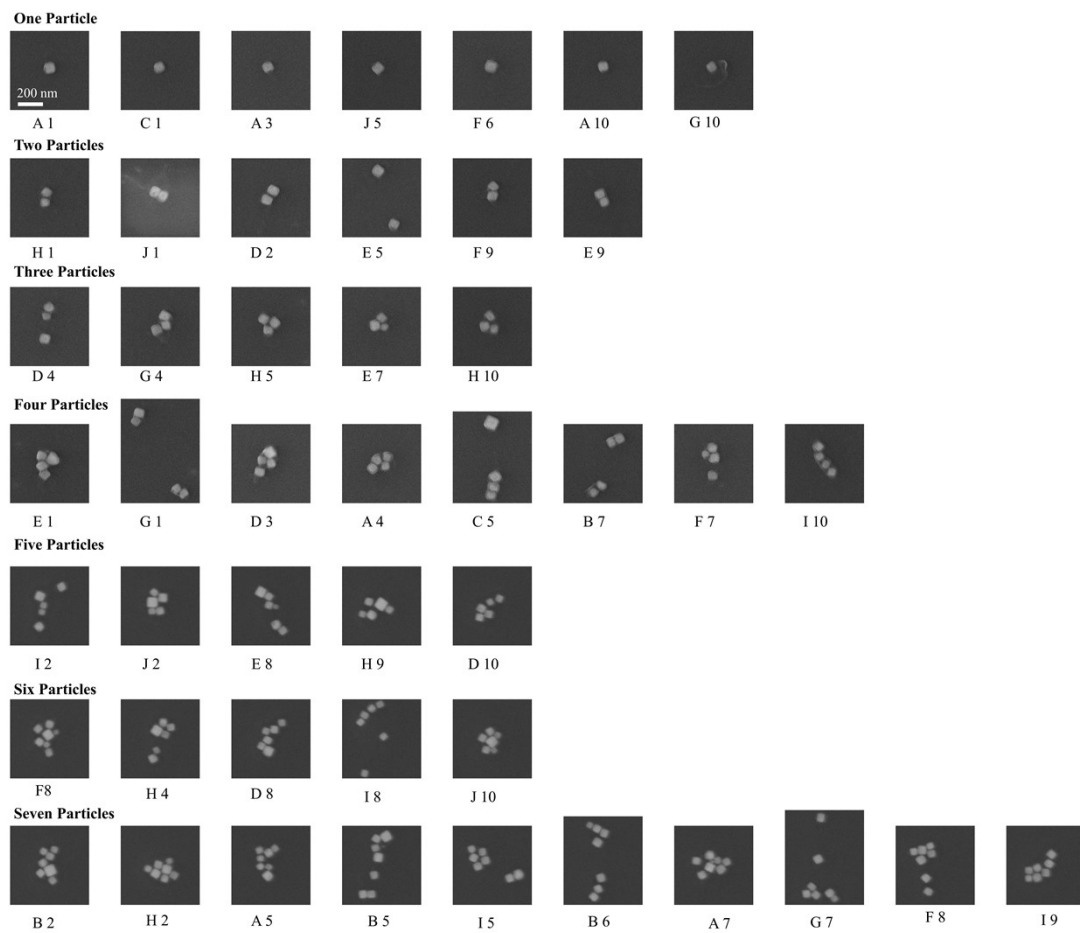
**Figure S2.** High-resolution SEM image of Ag@Au nanocubes shown in Fig.1d.



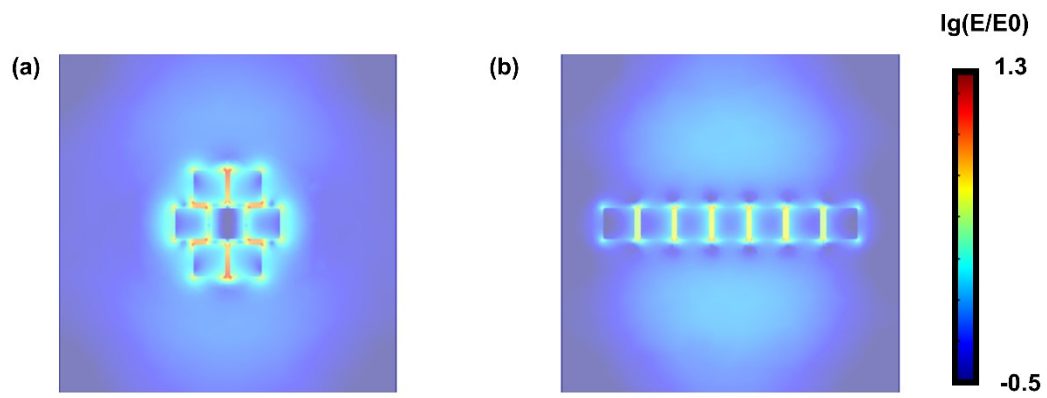
**Figure S3.** KFM image showing the distribution of surface potential on the substrate before (a) and after (b) one-week storage.



**Figure S4.** TEM images of Au nanoparticles



**Figure S5.** The SEM images and their corresponding number of all the counted clusters.



**Figure S6.** Simulation results showing the electric field distribution of the agglomerated clusters (a) and the chain-shaped clusters (b). The incident light wavelength was 532 nm.