Electronic Supplementary Material (ESI) for CrystEngComm.

Supporting Information

Digestive Ripening Mechanism Investigation in a Classical Lee-Meisel Method based on *in situ* UV–vis spectra

Liang Yu,[a] Hongjun You,*[a,b] Qifan Zhang,[b] Lingling Zhang,[b] and Jixiang Fang*[b]

a *School of Science, Xi'an Jiaotong University, Xi'an, Shaanxi 710049, China*

b *China Key Laboratory of Physical Electronics and Devices of Ministry of Education, School of Electronic and Information Engineering, Xi'an Jiaotong University, Xi'an, Shaanxi 710049, China*

Synthesis of Ag nanoparticles

The Ag nanoparticles were synthesized according to the Lee-Meisel method. Typically, 50 ml $AgNO_3$ aqueous solution (1 mM) in a conical flask was heated to boiling under stirring by magnetic bar. Following, 0.4 ml sodium citrate aqueous solution (100 mM) was injected into the boiling solution rapidly. The solution was turned to bright yellow within 3 min after the injection of sodium citrate, and then turned to taupe, and last turned to transparent red brown. After reaction of 30 min, the solution cooled down to room temperature and the product was washed 3 times with deionized water.

Characterization

The morphologies of the Ag nanoparticles was characterized using the field-emission scanning electron microscopy (SEM) (JEOL JSM-7000F) at an accelerating voltage of 20 kV and transmission electron microscopy (TEM) (JEOL JEM-2100) at an accelerating voltage of 200 kV. The ultraviolet-visible spectra were taken by Agilent Cary 60 spectrophotometer.

MD Simulation method

The MD simulation was performed in the Forcite package with the PCFF30 force field similar with our previous report.[1,2] The configurations of Ag nanoparticles was optimized with the PCFF30 force field which was based on the *ab initio* principle and empirical parameters.[3,4] The geometry optimizations were defined to be converged under the following criteria: the energy tolerance being less than 2.0×10^{-5} kcal mol^{-1} and the maximum displacement being less than 1.0×10^{-5} Å using a smart algorithm.

FDTD simulation method

The excitation spectra of the Ag NPs with four morphologies were calculated respectively using the finite-difference time-domain (FDTD) method. Four models were built and their geometric parameters are shown in Fig. S1. Model A shown in Fig. S1a is spherical Ag NP with 25 nm in diameter. Model B shown in Fig. S1b is triangular Ag nanoplate with 25 nm thickness and 60 nm length of side. With the prolonging of reaction time, the angles of the triangular nanoplate are gradually etched and its shape correspondingly transform to truncated triangle nanoplate (model C) and subsequently to approximate cylinder nanoplate (model D) which are shown in Fig. S1c-d respectively. The 3D model, 3D simulation area and uniform mesh were used. A total-field scattered-field source was used as the incident light. The source of light is in the uniform grid. The incident light propagates backward the z-axis and polarized along the y-axis as shown in Fig. S1a-d. The pink arrows indicate the direction of the incident light and the blue arrows indicate the polarized direction of the incident light. The wavelength range of incident light is 300 nm - 700 nm.

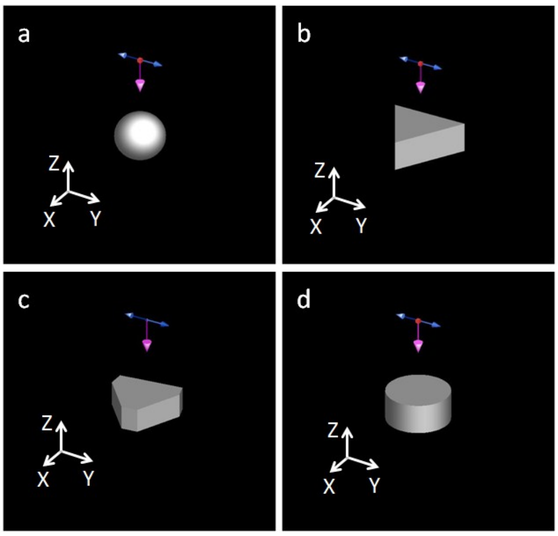

Fig. S1 Geometry models of Ag NPs. (a) Spherical Ag NP with 25 nm in diameter. (b) Triangular Ag nanoplate with 25 nm thickness and 60 nm length of side. (c) Polygon Ag nanoplate with 25 nm thickness. (d) Approximate cylinder Ag nanoplate with 25 nm thickness.

References

1. Z. Liu, F. L. Zhang, Z. B. Yang, H. J. You, C. F. Tian, Z. Y. Li and J. X. Fang, J. Mater. Chem. C, 2013, 1, 5567.

2. Z. B. Yang, L. Zhang, H. J. You, Z. Y. Li and J. X. Fang, Part. Part. Syst. Charact., 2014, 31, 390.

3. H. Sun, S. J. Mumby, J. R. Maple and A. T. Hagler, J. Am. Chem. Soc., 1994, 116, 2978.

4. H. Sun, Macromolecules, 1995, 28, 701.