Electronic Supplementary Information (ESI)

Facile and Green Synthesis of Well-dispersed Au Nanoparticles in PAN Nanofibers by Tea Polyphenols

Han Zhu [b], MingLiang Du*[a,b] , MeiLing Zou [b], CongSheng Xu [b], Ni Li [a,b], YaQin Fu [a,b]

[a] *Key Laboratory of Advanced Textile Materials and Manufacturing Technology, Zhejiang Sci-Tech University, Ministry of Education, Hangzhou 310018, P. R. China; Tel: 86-571-86843255; E-mail:* du@zstu.edu.cn

[b] *Department of Materials Engineering, College of Materials and Textile, Zhejiang Sci-Tech University, Hangzhou 310018, P. R. China*

Morphology of AuNPs in aqueous solution and embedded in PAN nanofibers

The thickness of the TP layers around AuNPs embedded in PAN nanofibers is quite different with those in aqueous solution. Fig. 1S shows the AuNPs in aqueous solution and embedded in PAN nanofibers. The thicknesses of TP layers around AuNPs with and without PAN are about 0.5-1 nm and 2-3 nm, respectively. With the presence of PAN, the chelating interaction between gold and TP were affected, in addition, the viscosity of the precursor solution were also substantially increased which will restrain the diffusion of TP onto the surface of AuNPs. Consequently, the thickness of TP layer around AuNPs in PAN nanofibers is much thinner.

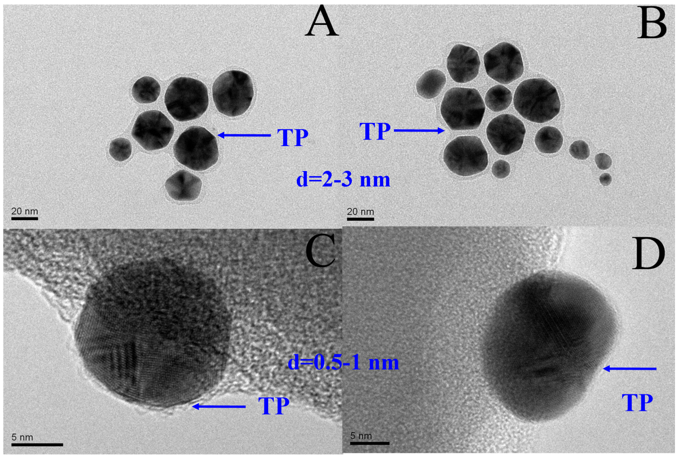

Fig. 1S TEM images of (A, B) AuNPs in aqueous solution and (C, D) AuNPs embedded in PAN nanofibers.

UV-vis spectra of TP heated for different time at 65°C

To confirm the reducibility of TP for Au(III), the UV-Vis spectra of TP heated for different time at 65°C were also testified. The UV-vis spectra of TP heated for different time at 65°C were shown in Fig. 2S and the absorption peaks around 275 nm have no changes, indicating that the heating (65 °C) is not sufficient to oxidize the

TP.[1]

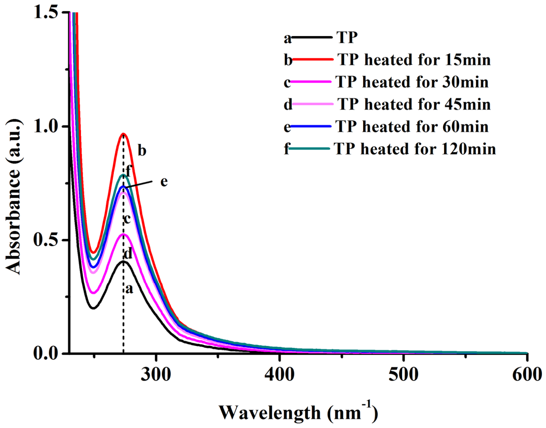

Fig. 2S UV-vis spectra of TP heated for different time at 65°C.

Morphology of AuNPs in PAN/DMF nanofibers precursor solution

The Morphology of AuNPs in PAN/DMF nanofibers precursor solution is shown in Fig. 3S. As shown in Fig. 4S, the mean particles size of AuNPs in PAN/DMF precursor solution is 5.6±1.2nm, which is similar to the diameter of AuNPs embedded in nanofibers.

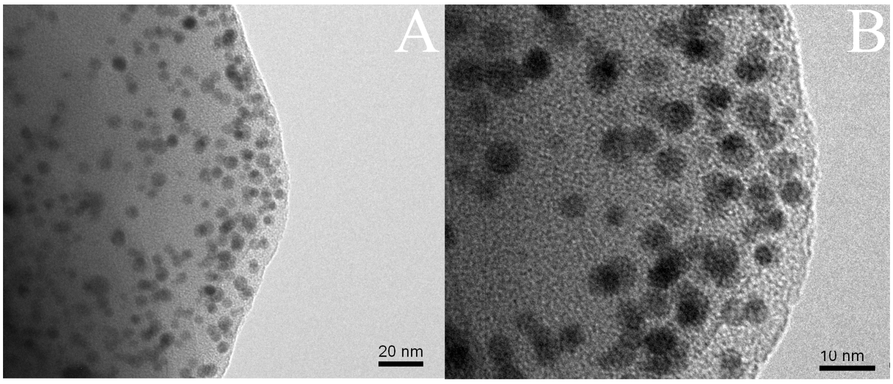

Fig. 3S TEM images of AuNPs in PAN/DMF solution with the reaction time of 60 min.

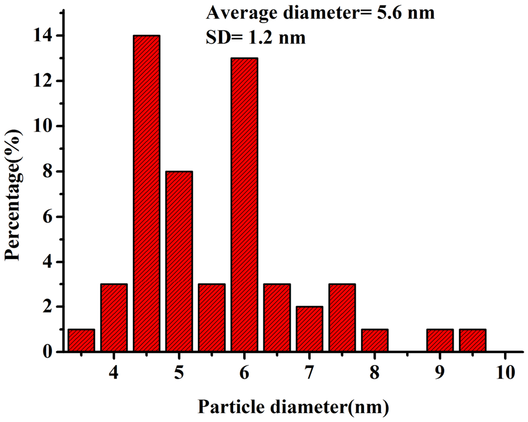

Fig. 4S The average diameter of AuNPs in PAN/DMF precursor solution.

FTIR spectra of TP and the solutions containing PAN, DMF and Au (III) solution after mixing with TP for 60 min and 200 min

The chemical changes of TP in the presence of PAN and DMF are verified by FTIR which are shown in Fig.5S. The color changes from gold yellow to orange red with increase of reaction time from 60 min to 200 min. The curve a in Fig. 5S showed the FTIR spectrum of the TP. The absorption band at 3352 cm^{-1} is ascribed to the phenolic hydroxyls of TP. But the band position of -OH in curve b and curve c changed to 3453 cm^{-1}, due to the strong hydrogen bond interaction between the phenolic hydroxyls of TP and the cyano groups.[2,4] The curve b and c showed the FTIR spectra of the mixture at different reduction time. It can be assigned as follows: 3453 cm^{-1} (-OH stretching in TP), 2936 cm^{-1} (C-H stretching in C-H and CH_2 groups), 2244 cm^{-1} (C≡N stretching), 1666 cm^{-1} (C=O stretching), 1439 cm^{-1} (C-H blending) and 1072 cm^{-1} (C-N blending).[3] Compared with curve a, the emerging absorption band at 2368 cm^{-1} in curve b and c is ascribed to the stretching vibration of C=O, suggesting the formation of the orthoquinone structure.[2,5] The absorption peaks at 1344 cm^{-1}, 1147 cm^{-1} and 1037 cm^{-1} which are belong to O-H in-plane bending vibration, O-H aromatic and C-O-H stretching vibration of phenolic hydroxyls in TP are covered by PAN and DMF, respectively.[3] The peak located at 3453 cm^{-1} decreased and became relatively narrow, which also implies the involvement of the O-H groups in the reduction of Au ions and the chelating effects between cyano groups and Au ions, resulting in the partial destruction of hydrogen bonds among TP molecules.[3-4]

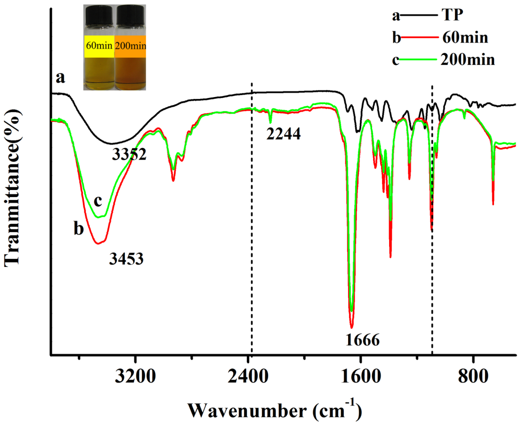

Fig. 5S The FTIR spectra of TP (curve a) and the solutions containing PAN, DMF and Au (III) solution after mixing with TP for 60 min (curve b) and 200 min (curve c).

FTIR spectra of AuNPs/PAN nanofibers

Fig. 6S shows that the absorption band at 3587 cm^{-1} is ascribed to the strong hydrogen bond interaction between the phenolic hydroxyls of TP and the cyano groups. Compared with curve a, the enhanced absorption band at 2378 cm^{-1} in curve b is ascribed to the stretching vibration of C=O, suggesting the formation of the orthoquinone structure.[2,5] The peak located at 3587 cm^{-1} in curve b decreased, which also implies the involvement of the O-H groups in the reduction of Au ions and the chelating effects between cyano groups and Au ions, resulting in the partial destruction of hydrogen bonds among TP molecules.[3-4]

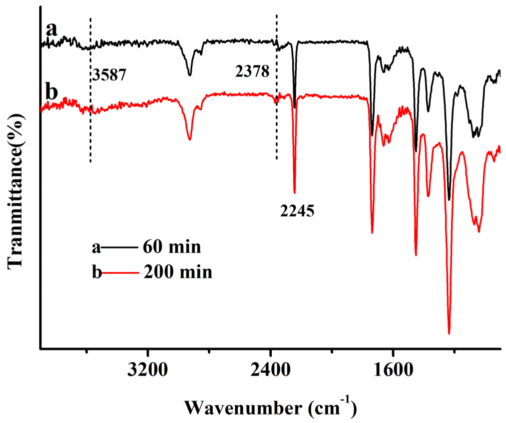

Fig. 6S FTIR spectra of AuNPs/PAN nanofibers: (a) reacted for 60 min, (b) reacted for 200min.

Morphology and diameter distribution of AuNPs/PAN nanofibers

The morphology and diameter distribution of AuNPs/PAN nanofibers are shown in Fig. 7S and 8S, respectively.

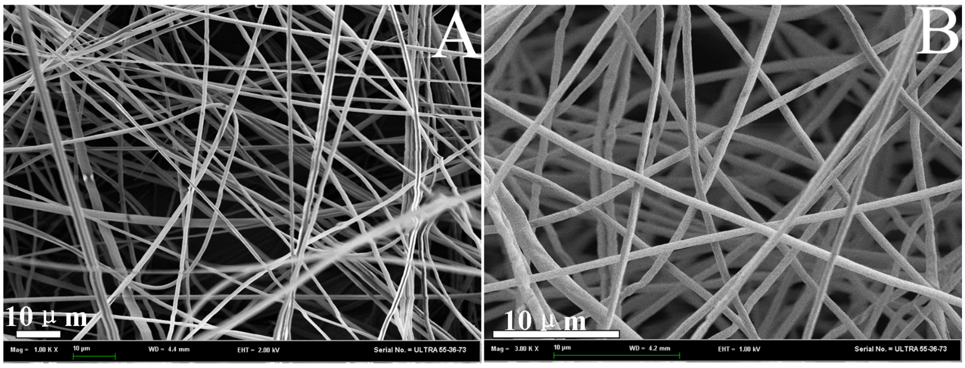

Fig. 7S FE-SEM images of AuNPs/PAN nanofibers with the reaction time of 60 min.

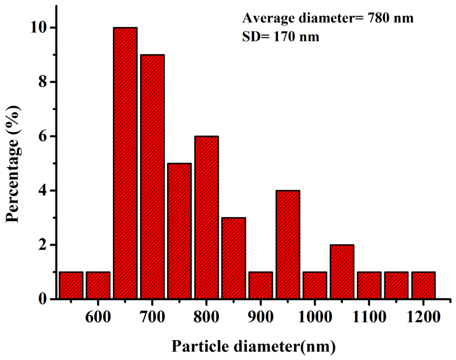

Fig. 8S The diameter distribution histograms of the AuNPs/PAN nanofibers with the reaction time of 60 min.

Reference

1 Y. D. Lei, Z. H. Tang, R. J. Liao and B. C. Guo, *Green Chem.*, 2011, **13**, 1655-1658.

2 Z. H. Tang, C. F. Zeng, Y. D. Lei, B. C. Guo, L. Q. Zhang and D. M. Jia, *J. Mater. Chem.*, 2011, **21**, 17111-17118

3 Z. R. Yue, K. R. Benak, J. W. Wang, C. L. Mangun and J. Economy, *J. Mater. Chem.*, 2005, **15**, 3142-3148

4 H. Wu, X. Huang, M. M. Gao, X. P. Liao and B. Shi, *Green Chem.*, 2011, **13**, 651-658.

5 R.J. Liao, Z. H.Tang, Y. D. Lei and B. C. Guo, *J. Phys. Chem. C*, 2011, **115**, 20740-20746.