[Supplementary Information]

Au@Pd core-shell nanocubes in finely-controlled sizes

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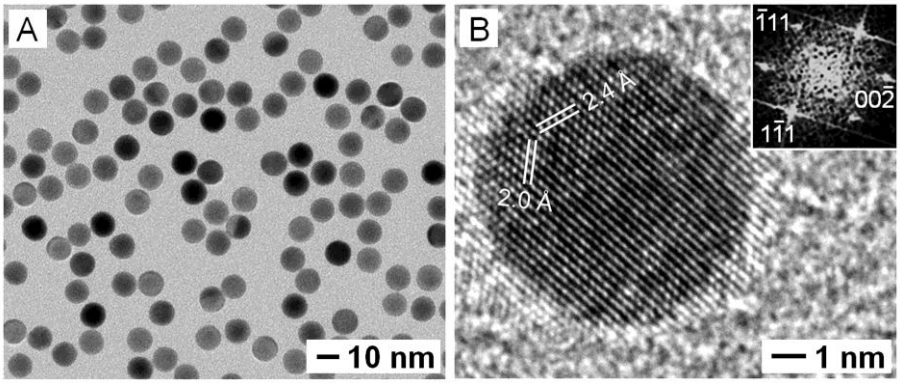


Fig. S1 (A) TEM image of the single-crystal spherical Au seeds with a diameter of 10.0 ± 0.3 nm. (B) HRTEM image taken from an individual Au seed and the corresponding FFT pattern (inset).

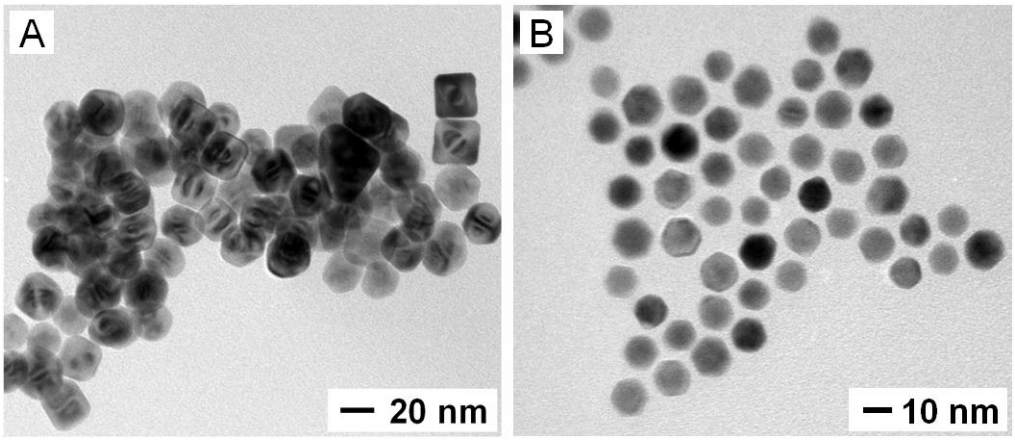


Fig. S2 TEM image of Au@Pd core-shell nanocrystals obtained using the standard procedure, except the reaction conducted at lower reaction temperature (19 ºC) (A) and for the use of much lower concentration of Na_2PdCl_4 (7.5 μM) (B).

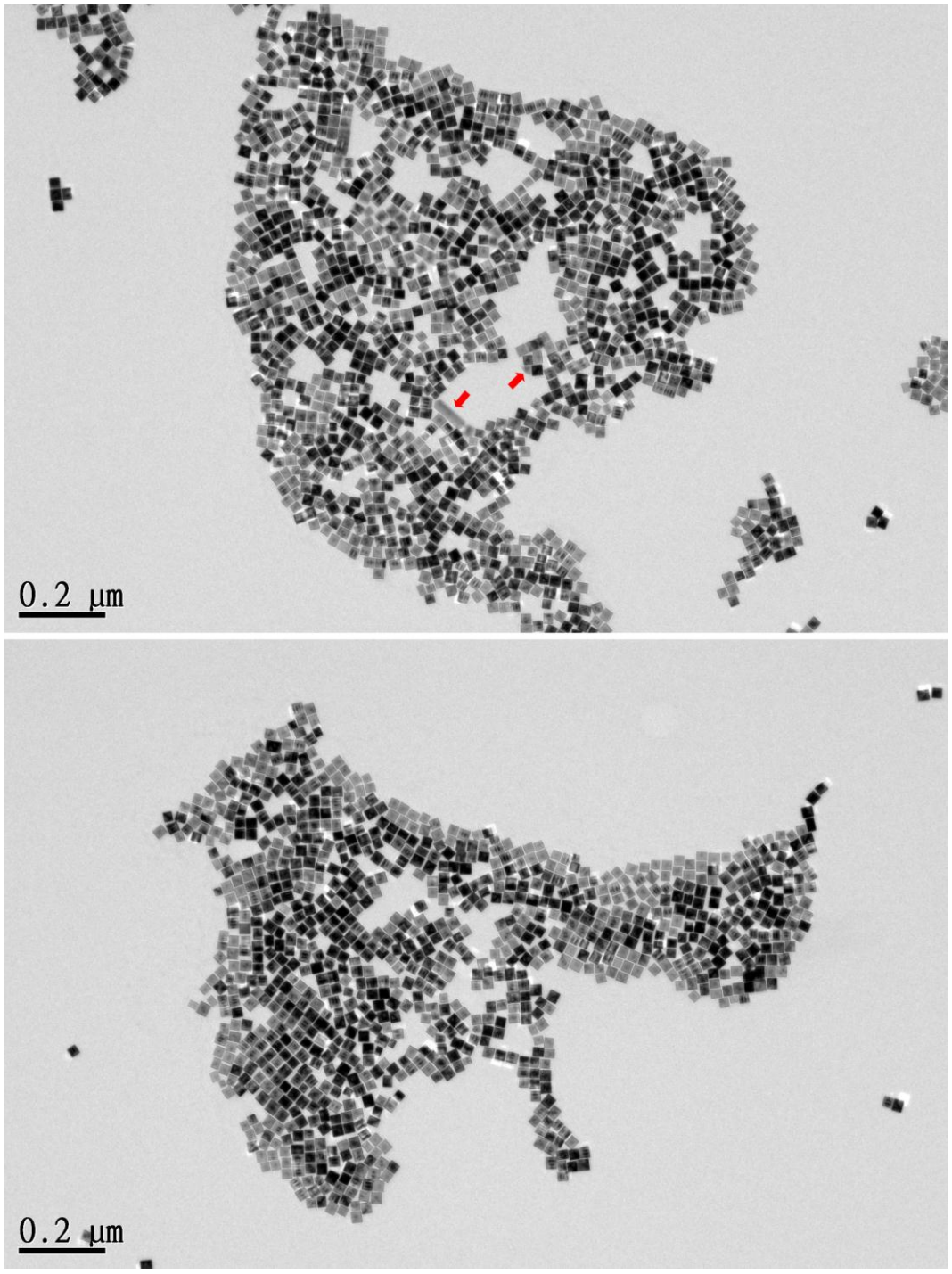


Fig. S3 Low-magnification TEM images of the Au@Pd core-shell nanocubes shown in Fig. 1. Red arrows indicate pentagonally twinned Au@Pd nanorod and single twinned Au@Pd bipyramid, respectively.

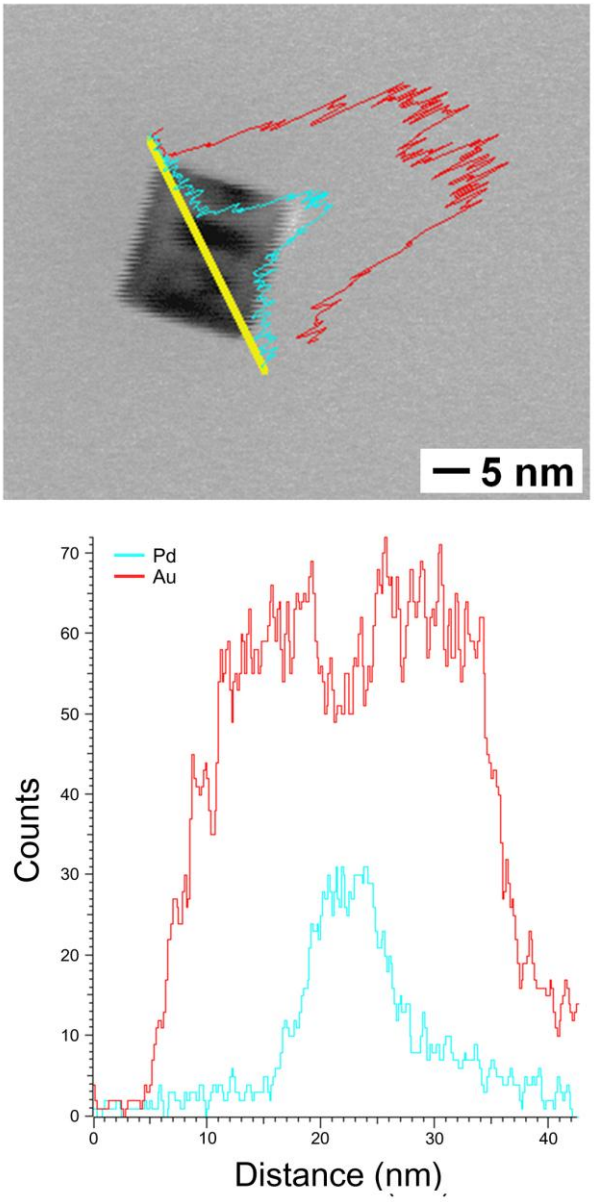


Fig. S4 TEM image of an individual Au@Pd core-shell nanocube obtained using the standard procedure and compositional line profiles of Au and Pd recorded along the diagonal indicated by a yellow line.

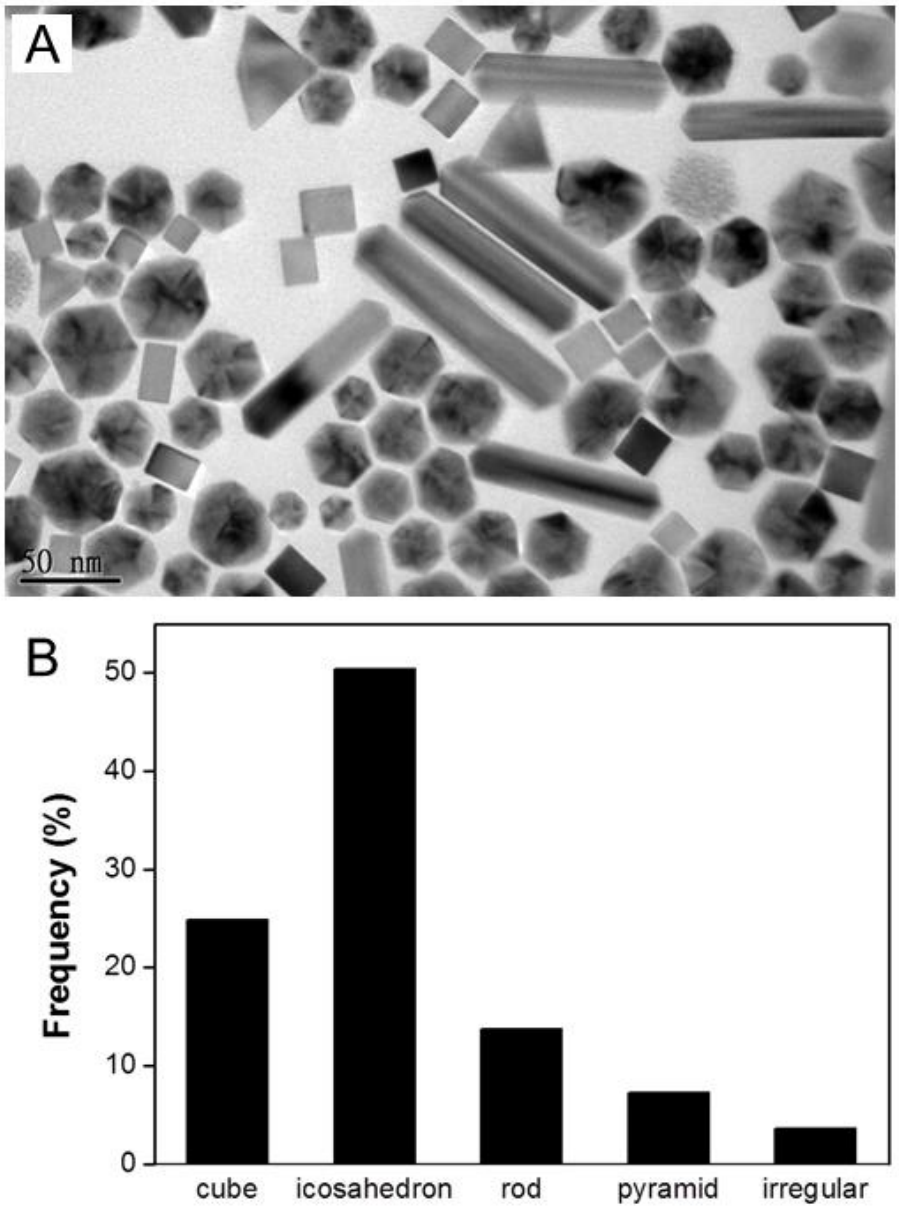
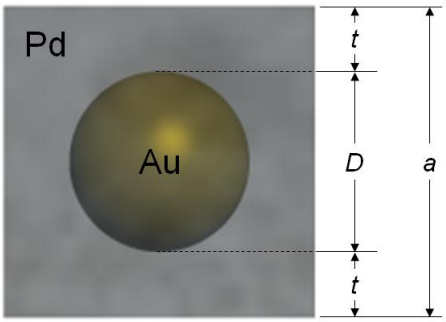


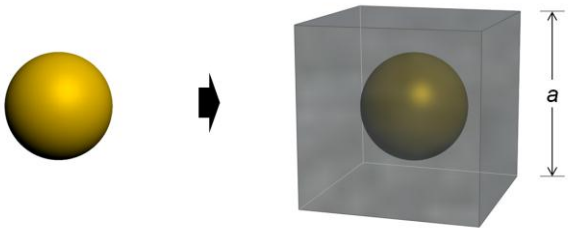
Fig. S5 (A) TEM image of Pd nanoparticles prepared using the standard procedure except the reaction without Au seeds in the reaction mixture and (B) histogram showing frequency of different shapes for the sample shown in Fig. S5A.

Definition of shell thickness of Au@Pd nanocube.



D, *a*, and *t* represent diameter of Au seed, edge length of the Au@Pd core-shell nanocube, and thickness of Pd shell, respectively.

Calculation of the expected sizes of resultant Au@Pd nanocubes.



The total volume and the edge length of Au@Pd core-shell nanocubes could be calculated using following equations,[S1]

$$V_{Au@Pd} = \frac{C_{Pd} \cdot V_{Pd} \cdot M_{Pd}}{D_{Pd}} + V_{Au}, \quad a = \sqrt[3]{V_{Au@Pd}}$$

,where *C*, *V*, *M*, *D*, and *a* represent concentration, volume, molar mass, density, and edge length, respectively. According to the above equations, the edge lengths of Au@Pd nanocubes obtained under different reaction conditions are summarizes in Table S1.

Table S1 Calculated edge lengths of Au@Pd core-shell nanocubes obtained using different concentrations of Na_2PdCl_4, or volumes of the Au seed suspension.

vol. of seed suspension (μL)	# of Au seeds ($\times 10^{12}$)	conc. of Pd (mM)	V_{Au} ($\times 10^{14}$, nm^3)	$V_{Au@Pd}$ ($\times 10^{16}$, nm^3)	$a_{Au@Pd}$ (nm)
50	1.57	0.023	8.22	0.20	10.9
50	1.57	0.038	8.22	0.28	12.1
50	1.57	0.075	8.22	0.48	14.5
50	1.57	0.225	8.22	1.28	20.1
50	1.57	0.375	8.22	2.07	23.6
50	1.57	0.525	8.22	2.87	26.3
50	1.57	0.750	8.22	4.07	29.6
50	1.57	1.50	8.22	8.05	37.2
50	1.57	2.25	8.22	12.0	42.5
30	0.942	0.375	4.93	2.04	27.9
100	3.14	0.375	16.4	2.16	19.0

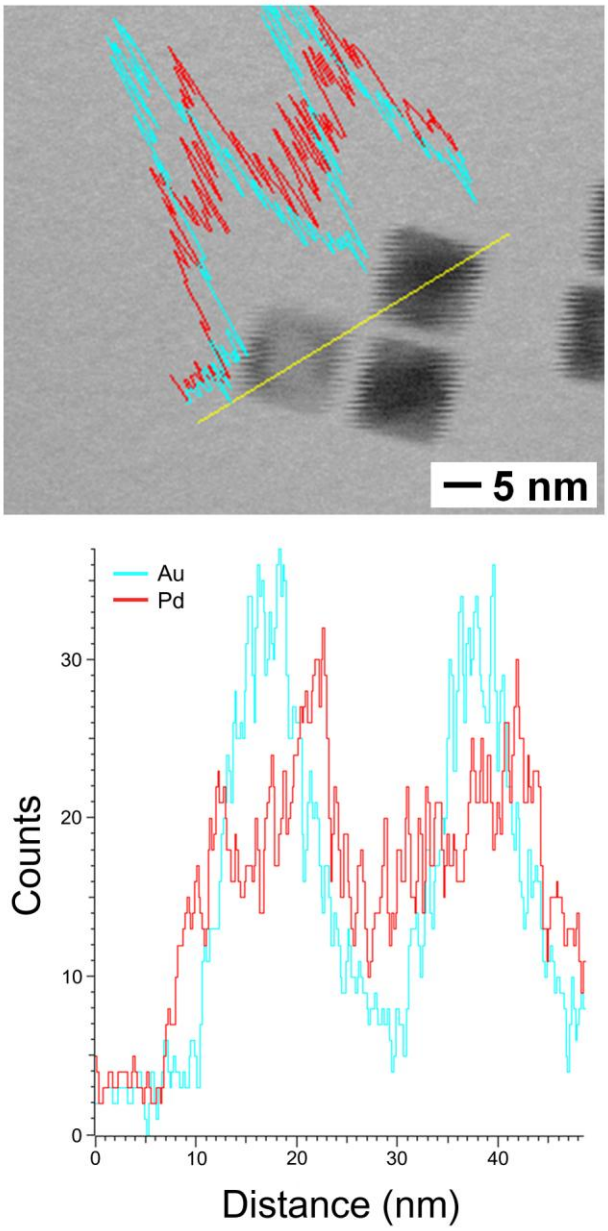


Fig. S6 TEM image of Au@Pd core-shell nanocubes shown in Fig. 2A and compositional line profiles of Au and Pd recorded along the diagonal indicated by a yellow line.

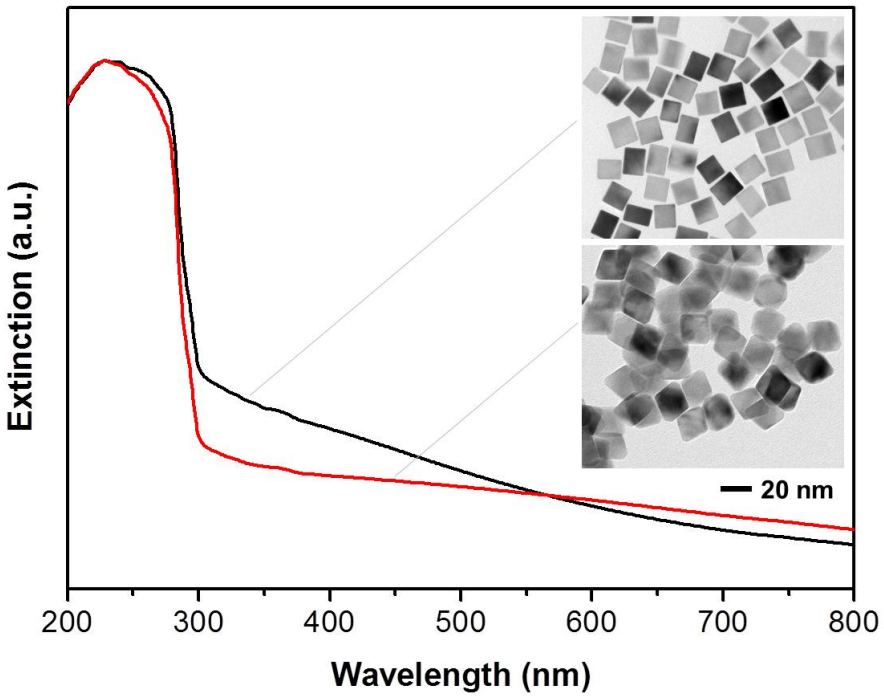


Fig. S7 UV-vis spectra of the Pd nanocubes (black) and the octahedra (red) and the corresponding TEM images (inset). The Pd nanocubes with an average edge length of 15.0 ± 1.7 nm were prepared by just following the procedure described in ref. S2. The Pd octahedra with an average edge length of 18.4 ± 1.1 nm were prepared by following the procedure described in the ref. S3 with a minor modification that a 60 mM CTAC aqueous solution was use instead of a 80 mM CTAC aqueous solution.

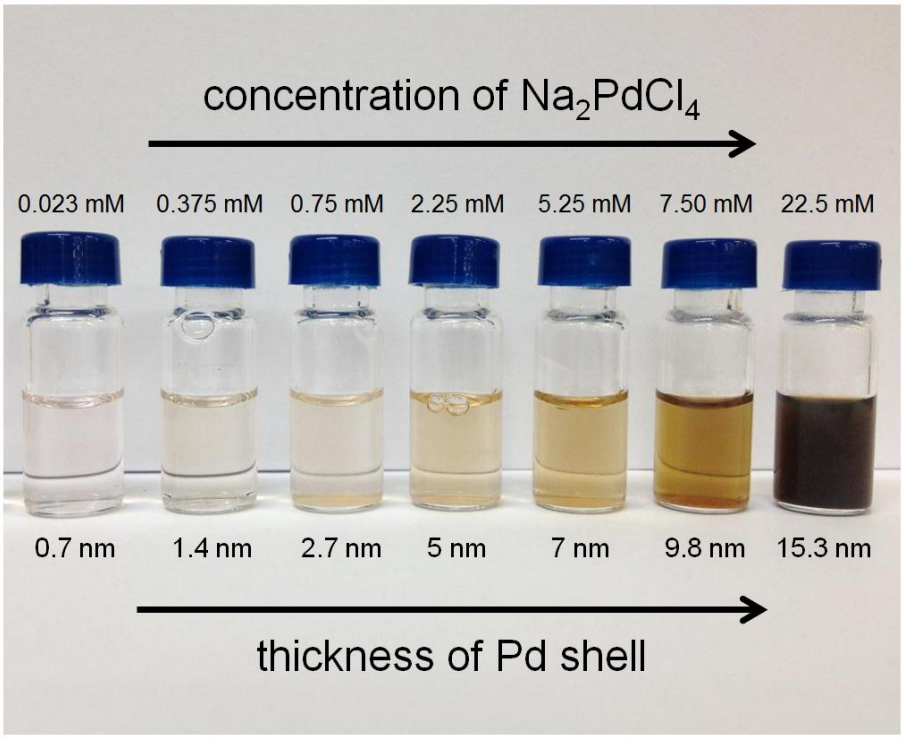


Fig. S8 Photograph of aqueous solutions containing the Au@Pd core-shell nanocubes with different thicknesses obtained under different concentrations of Na_2PdCl_4 while the amount of Au seeds kept the same.

References

[S1] F.-R. Fan, D.-Y. Liu, Y.-F. Wu, S. Duan, Z.-X. Xie, Z.-Y. Jiang, Z.-Q. Tian, *J. Am. Chem. Soc.*, 2008, **130**, 6949.

[S2] M. Jin, H. Liu, H. Zhang, Z. Xie, J. Liu, Y. Xia, *Nano Res.*, 2011, **4**, 83.

[S3] J. W. Hong, D. Kim, Y. W. Lee, M. Kim, S. W. Kang, S. W. Han, *Angew. Chem. Int. Ed.*, 2011, **50**, 8876.