Electronic Supplementary Material (ESI) for Journal of Materials Chemistry B

Size-controlled synthesis and characterization of CoPt nanoparticles using protein shells

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Supporting information

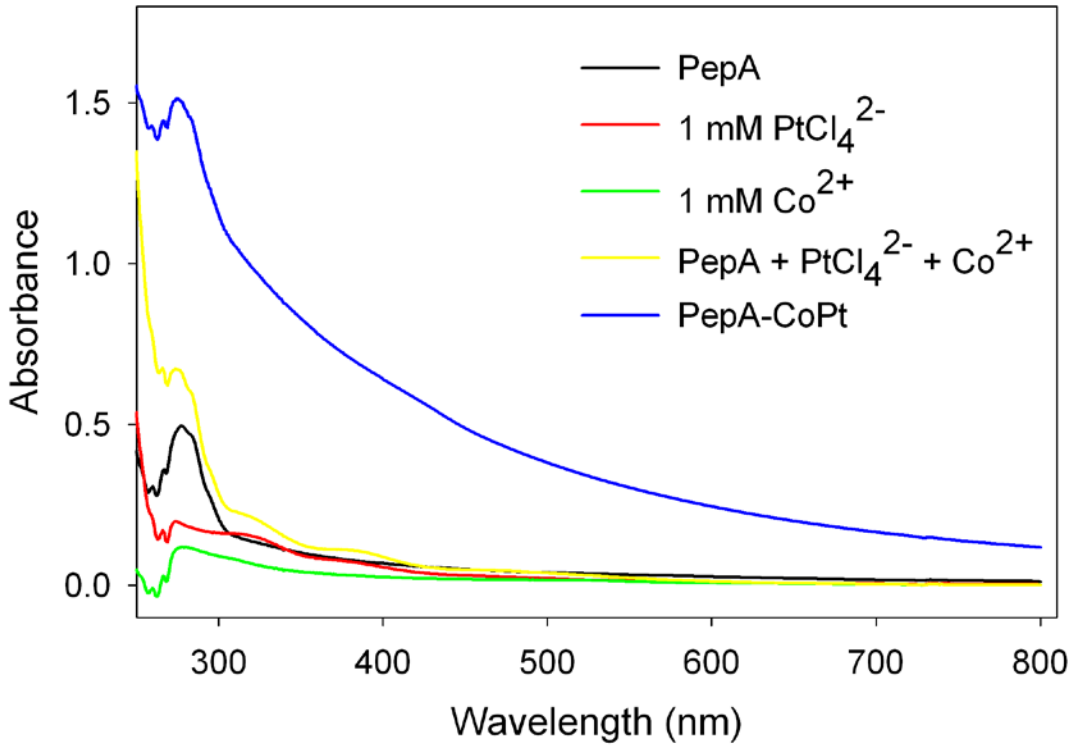


Fig. S1. UV/Vis spectra of PepA, Co and Pt precursors and PepA-CoPt complex. The spectra were recorded in the range of 250–800 nm. PepA-CoPt showed a broad absorption in UV-Vis region, but other samples did not show the absorbance at a visible wavelength region.

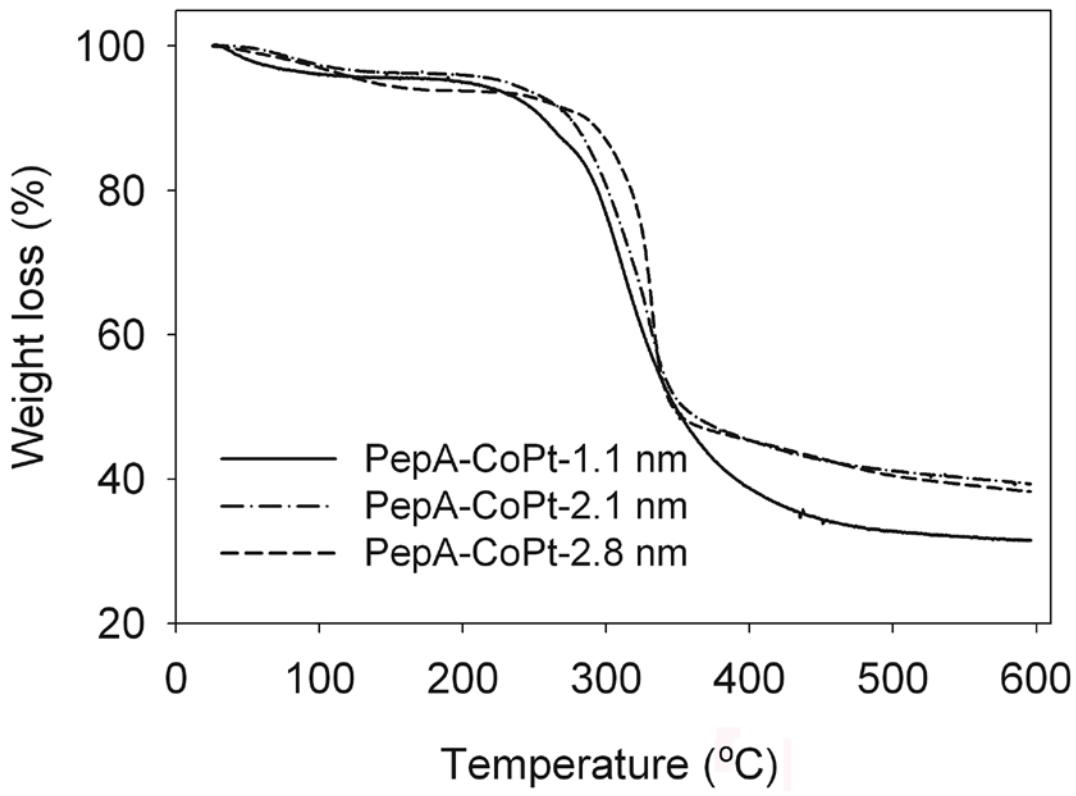


Fig. S2. Thermogravimetric analysis (TGA) recorded from the purified powders of PepA-CoPt complexes. PepA-CoPt complexes at 1.1, 2.1, and 2.8 nm sizes exhibited an overall weight loss of 64, 52, and 50 %, respectively. The weight loss was started observed at 240, 270, and 290 ^{o}C for 1.1, 2.1, and 2.8 nm, respectively. The weight loss is mainly due to decomposition of the encapsulated protein shell and the trapped solvent. The difference in the weight loss temperature is contributed by the amount of the protein shell, and consequently, correlated with the size of CoPt nanoparticle in the complex. Based on these results, the temperature at 300 ^{o}C was selected as an annealing temperature for the removal of PepA shell from the PepA-CoPt complex.

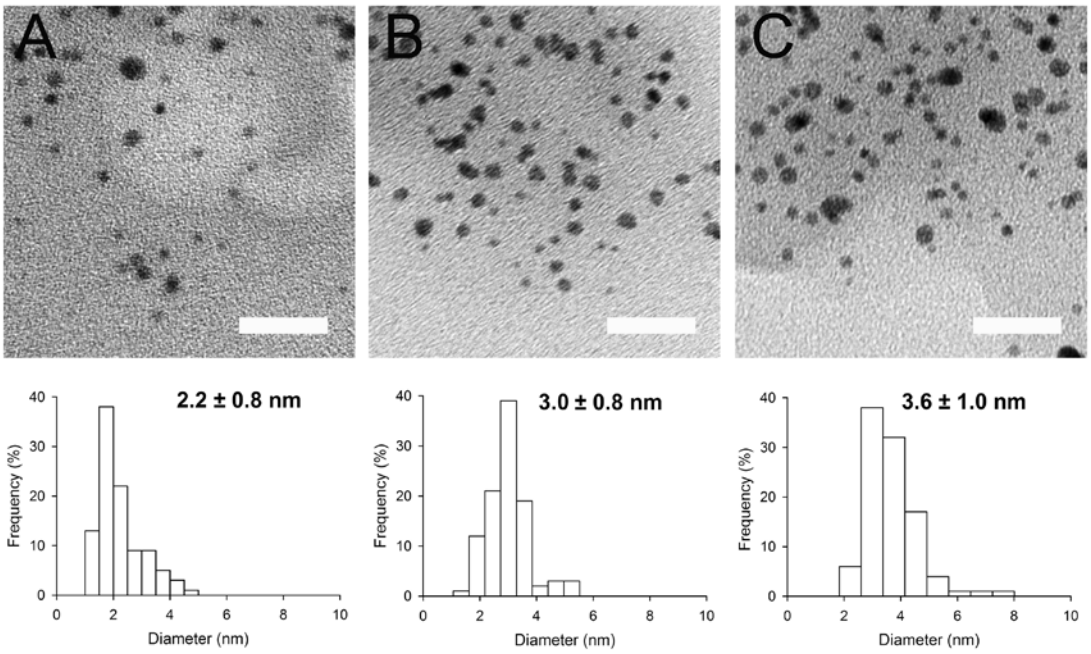


Fig. S3. TEM images of CoPt NPs annealed at 300 ^{o}C in 1 hour under nitrogen atmosphere to remove PepA shells. The sizes of CoPt NPs after annealing reached 2.2 ± 0.8 nm (A), 3.0 ± 0.8 nm (B), and 3.6 ± 1.0 nm (C) when Co:Pt precursors were incubated with PepA in the as-prepared samples at molar ratios of 50:50:1, 500:500:1, and 1500:1500:1, respectively. The size distribution histograms shown in the below panel of each sample showed the mean diameter and standard deviation of 100 individual particles. Each scale bar represents 20 nm.

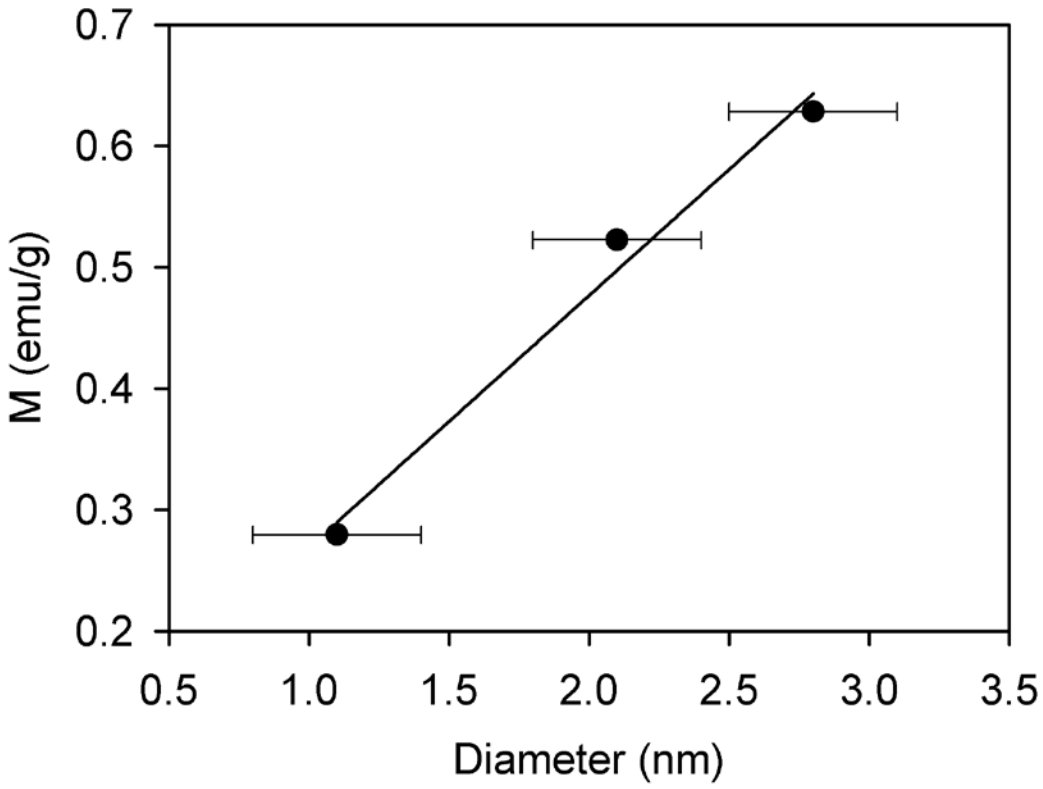
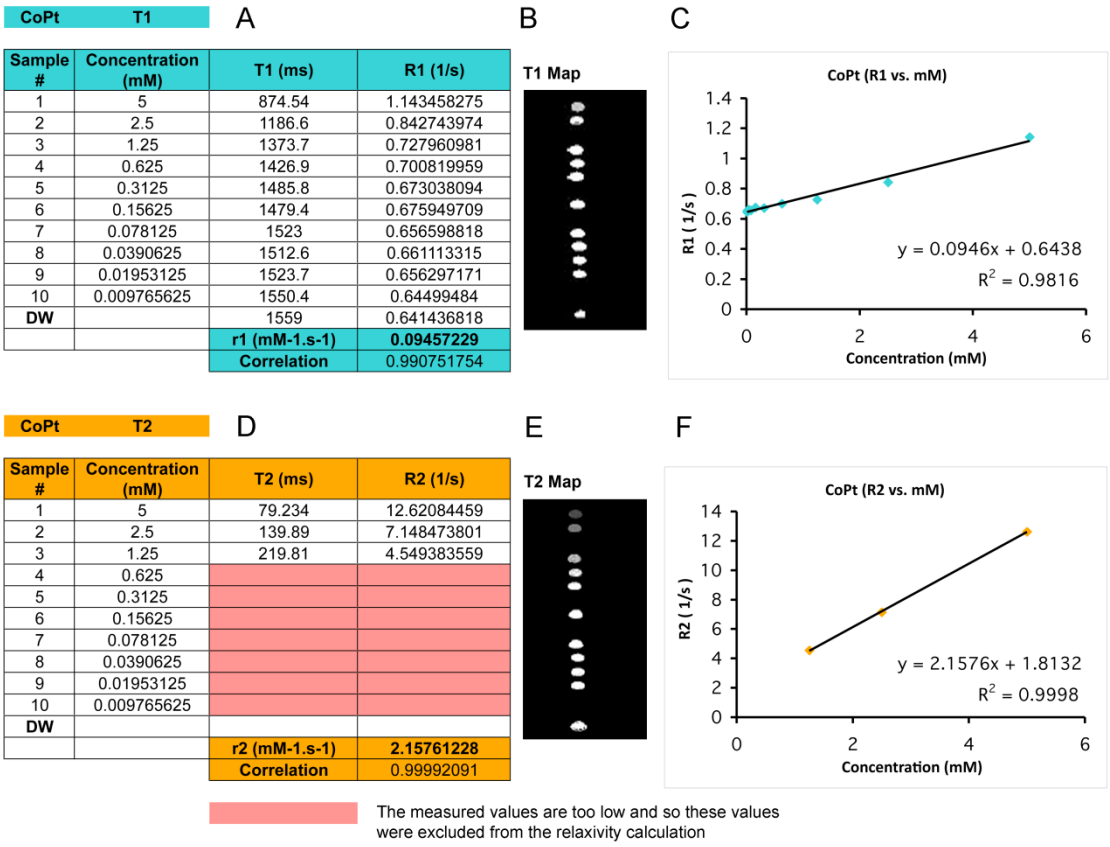


Fig. S4. Magnetization of PepA-CoPt NPs as a function of the size of CoPt NPs encapsulated by PepA shells. The magnetic properties of the as-prepared PepA-CoPt NPs of different sizes were measured at 5 K and with the magnetic field of 5 T.



Sample #	Concentration (mM)	T1 (ms)	R1 (1/s)
1	5	874.54	1.143458275
2	2.5	1186.6	0.842743974
3	1.25	1373.7	0.727960981
4	0.625	1426.9	0.700819959
5	0.3125	1485.8	0.673038094
6	0.15625	1479.4	0.675949709
7	0.078125	1523	0.656598818
8	0.0390625	1512.6	0.661113315
9	0.01953125	1523.7	0.656297171
10	0.009765625	1550.4	0.64499484
DW		1559	0.641436818
		r1 (mM-1.s-1)	0.09457229
		Correlation	0.990751754

Sample #	Concentration (mM)	T2 (ms)	R2 (1/s)
1	5	79.234	12.62084459
2	2.5	139.89	7.148473801
3	1.25	219.81	4.549383559
4	0.625		
5	0.3125		
6	0.15625		
7	0.078125		
8	0.0390625		
9	0.01953125		
10	0.009765625		
DW			
		r2 (mM-1.s-1)	2.15761228
		Correlation	0.99992091

Fig. S5. Magnetic resonance (MR) relaxation of PepA-CoPt. Each set of 10 MR images was used to calculate the T_1 (A-C) and T_2 (D-E) relaxivity values of the 2.1 nm PepA-CoPt. Panel A and D present the concentrations of PepA-CoPt NPs, with the numbers corresponding to the MR images recorded in the panels (B) and (E) from top to down for T_1 and T_2 values, respectively. The specific relaxivities (r_1 and r_2) of PepA-CoPt were calculated from the plot of T_1^{-1} (C) and T_2^{-1} (F) *vs*. concentration of PepA-CoPt. T_1 and T_2 relaxivities calculated from the MR images were 0.1 $mM^{-1}s^{-1}$ and 2.2 $mM^{-1}s^{-1}$, respectively. Distilled water (DW) was used as a control.

Table S1. Percentage of total carbon weight in CoPt NP samples.

Theoretical precursor loading molar ratio (Co:Pt:PepA)	As-prepared PepA-CoPt NPs		Annealed CoPt NPs
	Theoretical result* (%)	Experimental result (%)	Experimental result (%)
50:50:1	52.89	45.56	54.68
500:500:1	48.69	38.13	41.42
1500:1500:1	43.86	26.35	37.89

*The theoretical results were calculated considering the molecular weight of protein, atomic weight of metals, and number of metal atoms in one protein shell (24 subunits of PepA). The number of metals ions was estimated using the average size and composition of Co and Pt ions determined from TEM and ICP-MS, respectively (Table 1).