Electronic Supplementary Information (ESI)

Size-controlled Synthesis of Pd Nanocrystals Using a Specific Multifunctional Peptide

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1. Experiment procedures

A. Selection of peptide sequence (biopanning)

Peptide selection was carried out with M13 Phage Display library through the biopanning procedure. Ph.D.-7mer peptide library from New England Biolabs was used. The Pd wire (0.5 mm in diameter, 99.99% pure, from Sigma Aldrich) was incubated in10 µl of 2x10¹¹ library phages which were dilute in 990 µl of TBS containing 0.1% TWEEN-20, to reduce phage-phage interactions on the surface. After rocking for 1 h at room temperature, the surfaces were washed with 10 exposures to TBS containing 0.1% TWEEN-20, pH 7.5, and increasing TWEEN-20 concentrations to 0.3% and 0.5% for the following two rounds. The phages bounded on Pd surface were eluted from the surface by adding glycine-HCl (pH 2.2) with gently rocking for 8 min, transferred to a fresh tube and then neutralized with Tris-HCl (pH 9.1). The eluted phage were amplified by infecting Escherichia coli ER2738 in 25 mL of lysogeny broth (LB) and allowed to grow for 4.5 hours in an incubating shaker. The resulting phage were then purified and used for next round of biopanning. The phage elute at the third round of biopanning was plated on LB XGal/IPTG plates. 10 blue plaques were then picked from the plate and DNA sequenced to obtain their peptide sequence. In this study, the selected peptide, QQSWPIS, appeared four times among ten colonies.

B. Peptide Synthesis

All used peptides were synthesized employing standard F-moc solid phase peptide synthesis (SPPS) protocol with a peptide synthesizer from C.S.Bio Co, purified by HPLC method and tested by liquid chromatography mass spectrometry (LC-MS). The used peptides were confirmed to have a high purity and valid molecular mass. The molecular structure and the characterization with LC-MS of Q7 are shown in Figure S1.



Figure S1 (a) Molecular structure of the selected peptide molecular, Q7. (b) LC chromatogram of 1 μ g ml⁻¹ of Q7 peptide solution. (c) MS spectrum of the elute sample at 22 min.

C. Pd NCs Synthesis

All reactions were carried out in aqueous solution at room temperature. The total volume of solution in a vial is 5 ml. Three vials containing 1 ml of 5 mM Na₂PdCl₄, 250 μ l of 2 mg ml⁻¹ peptide solution and different volume of de-ionized water, 3.7 ml, 3.65 ml and 3.6 ml for reacting with NaBH₄. 50 μ l, 100 μ l and 150 μ l of 50 mM NaBH₄ were injected to three pre-prepared solutions to result in 0.5 mM, 1 mM and 1.5 mM of NaBH₄ in reaction solutions. The final peptide concentration was 100 μ g/ml and the final concentration of Na₂PdCl₄ was 1 mM. The color of the solutions changed from yellow to brown as soon as the injection of NaBH₄. Reaction solution was taken by pipetting droplets of solution

on parafilm and upside down TEM grids on the droplets waiting for 1 minute. The grids were rinsed with de-ionized water for 30 s and dried.

D. Seeding growth

Three seed solutions containing three-sized of Pd NCs were prepared by injecting 50 μ l, 100 μ l and 150 μ l of 50 mM NaBH₄ into precursor/peptide solutions and reacting for 1 hour. For each seed solution, 50 μ l, 100 μ l and 200 μ l of growth solution (5 mM of Na₂PdCl₄) were added respectively into the seed solutions and kept vigorous stirring for one hour. After reaction, the same TEM sample preparation method was used.

E. Characterization

Transmission Electron Microscopy (TEM) and High-Resolution TEM (HRTEM) characterization Pd NCs were imaged on Philips CM120 with a 120 kV operation voltage. HRTEM of Pd NCs was conducted on FEI TITAN with a 300 kV operation voltage.

2. TEM images of W- and Q7- incubations



Figure S2 TEM images of the obtained Pd from the incubations (a) W in Na₂PdCl₄ (b) Q7 in Na₂PdCl₄.



Figure S3 TEM images of the obtained Pd NCs at 10 min from the reactions with the concentration of NaBH₄: 1.5 mM (a), 1 mM (b) and 0.5 mM (c) at 10 min.