Electronic Supplementary Material (ESI) for Journal of Materials Chemistry

Supporting Information

Specific functionalization of CTAB stabilized anisotropic gold nanoparticles with polypeptides for folding-mediated self-assembly

Yusong Wang,[a,b] Daniel Aili,[a,c] Robert Selegård,[c] Yeeyan Tay,[b] Lars Baltzer,[d] Hua Zhang,[a,b] Bo Liedberg*[a,c]

[a] *Centre for Biomimetic Sensor Science, Nanyang Technological University, 50 Nanyang Drive, Singapore 639798.* [b] *School of Materials Science and Engineering, Nanyang Technological University, 50 Nanyang Avenue, Singapore 639798.*[c] *Division of Molecular Physics, Department of Physics, Chemistry and Biology, Linköping University, 581 83 Linköping, Sweden.* [d] *Department of Biochemistry and Organic Chemistry, Uppsala University, BMC, Box 576, 751 23 Uppsala, Sweden.*

Peptide synthesis: The polypeptides JR2EC, (NAADLEKAIEALEKHLEAKGPCDAAQLEKQLEQAFEAFERAG), and JR2KC (NAADLKKAIKALKKHLKAKGPCDAAQLKKQLKQAFKAFKRAG), were synthesized on a Pioneer automated peptide synthesizer (Applied Biosystems) using standard fluorenylmethoxycarbonyl (Fmoc) chemistry. The crude products were purified by reversed-phase HPLC on a semi-preparative HICHROM C-8 column and identified by MALDI-TOF mass spectrometry. In order to obtain $JR2KC_2$, lyophilized peptide monomers (1 mM) were dissolved in 0.1 M ammonium bicarbonate buffer pH 8, aerated for 90 minutes and incubated at 4^{o} C for at least 24 hours before use. Complete oxidation was confirmed using a standard Ellman´s test for determination of free thiols.[1]

High resolution TEM:

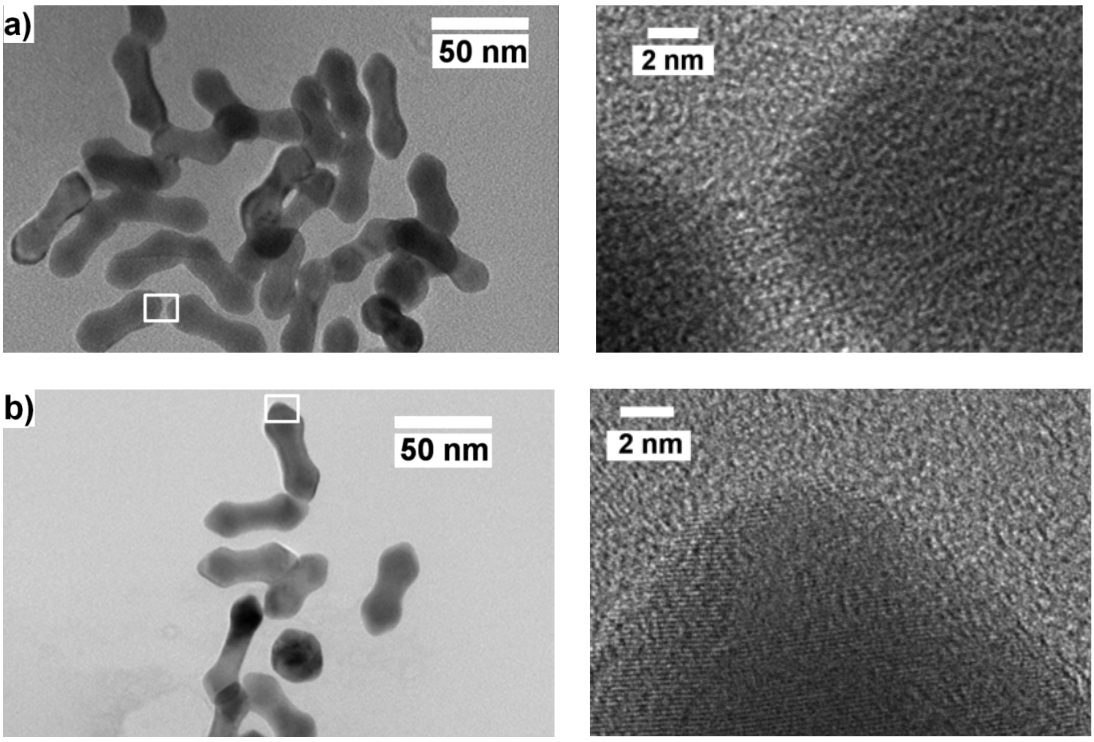


Figure S1. HR-TEM image of the arrowhead nanorods before (a) and after (b) Au layer growth. Insets are the enlarged area of the gold particles in a) as indicated by the white box.

FT-IR: FT-IR spectra was recorded of soloution casted multilayers of JR2KC modifed nanorods on CaF_2 windows. In addition to the extensive washing after peptide immobilization, two additional centrifugation steps were carried out and the buffer was replaced by ultrapure water in order to elliminate any contributions from non-immobilized peptides. Spectra were recorded using a Vertex 70 instrument (Bruker Corp.) with a 2 cm^{-1} resolution. A three-term Blackmann-Harris apodization function was applied to the interferograms before Fourier transformation.

The amide I (C=O stretching) and amide II (C-N-H stretching and bending) bands apperead at 1655 and 1544 cm^{-1}, respectively, which is in excellent agreement with previously published data of the same peptide without the Cys residue (1656 and 1545 cm^{-1}).[2] Additional bands at 1578 and 1412 cm^{-1}, most likely correspond to the assymetric $–C=COO^-$ and symmetric $–CO_2$ streching vibrations of remaining actetate buffer, respectively.[3]

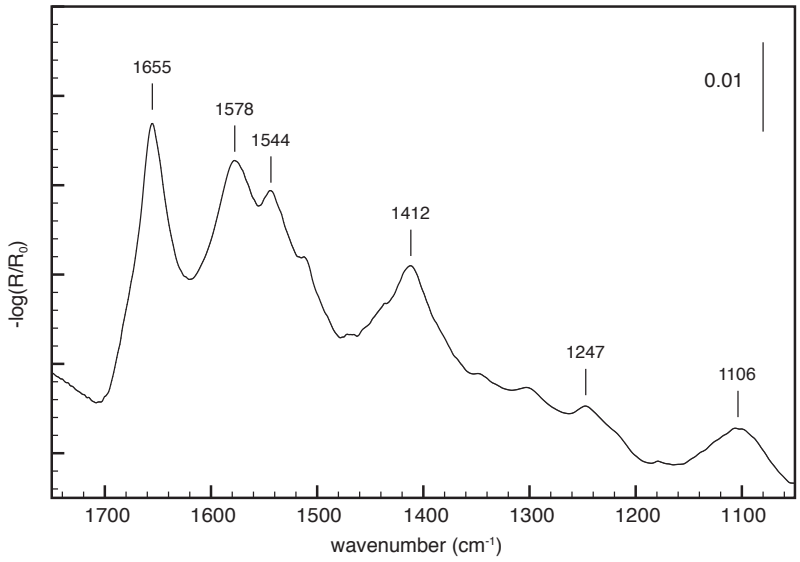


Figure S2. FT-IR spectrum of JR2KC modified gold nanorods.

FESEM-TED:

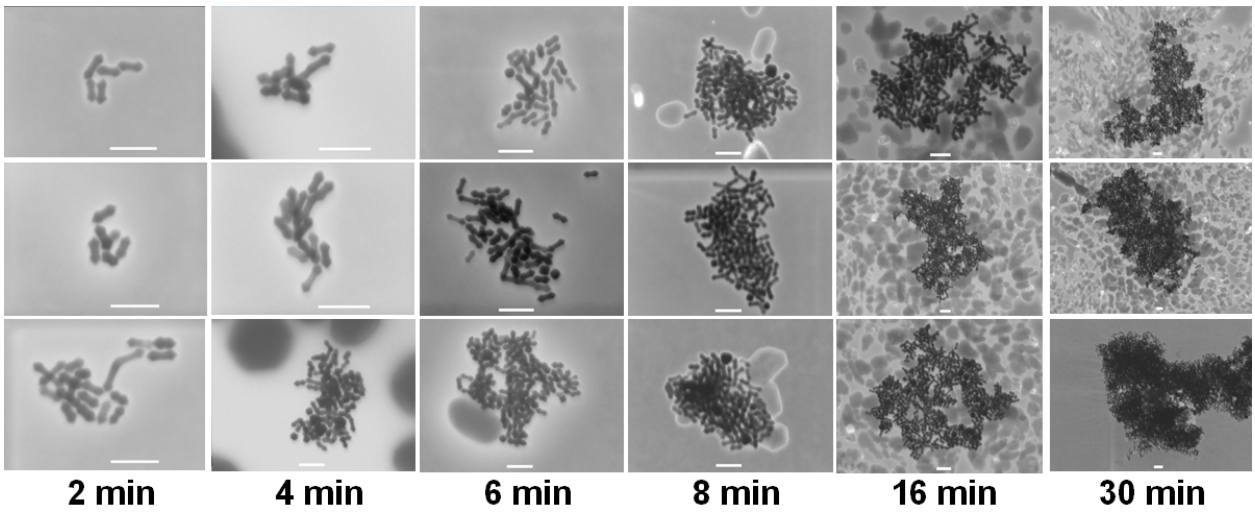
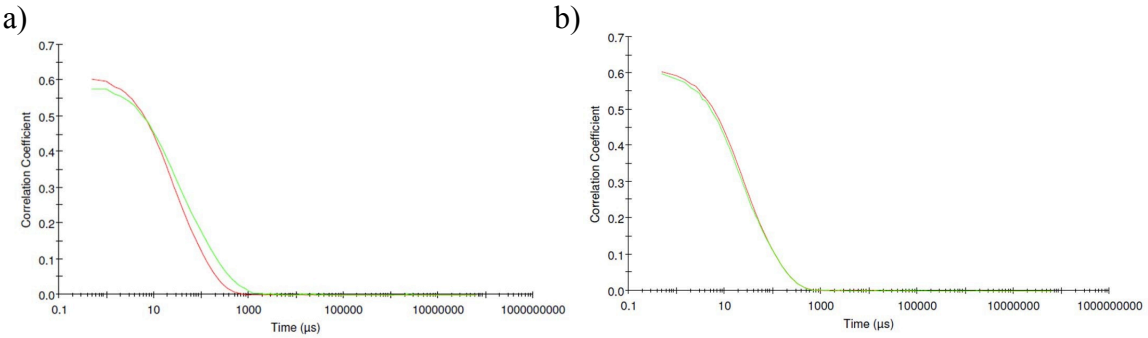
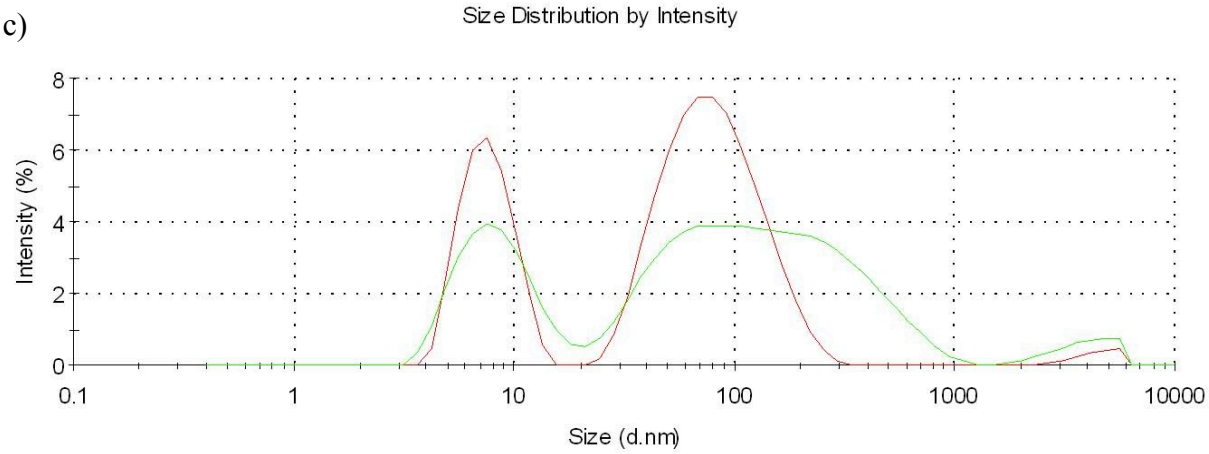


Figure S3. Representative FESEM-TED images of the assembly of JR2KC functionalized arrowhead gold nanorods after addition of 2 µM $JR2EC_2$ at different time points during the assembly in three different samples. Scale bars: 100 nm.

Dynamic light scattering (DLS): DLS was carried out on a Malvern Nano Sizer using low volume cuvettes (ZEN0112). Typically, 18 µL JR2KC functionalized NR stock solution (2.4 nM) was dispersed in 400 µL fresh HBS-EP buffer (GE Healthcare, 0.01M HEPES, pH 7.4, 0.15 M NaCl, 3 mM EDTA, 0.005% surfactant P20) followed by DLS measurements. Peptides were added to the solution while mixing until the final polypeptide concentration was ~ 2.3 µM. DLS was measured before and 30 minutes after addition of $JR2EC_2$ or $JR2ECref_2$. The same procedure was used for both $JR2EC_2$ and $JR2EC_{ref2}$.



c)



d)

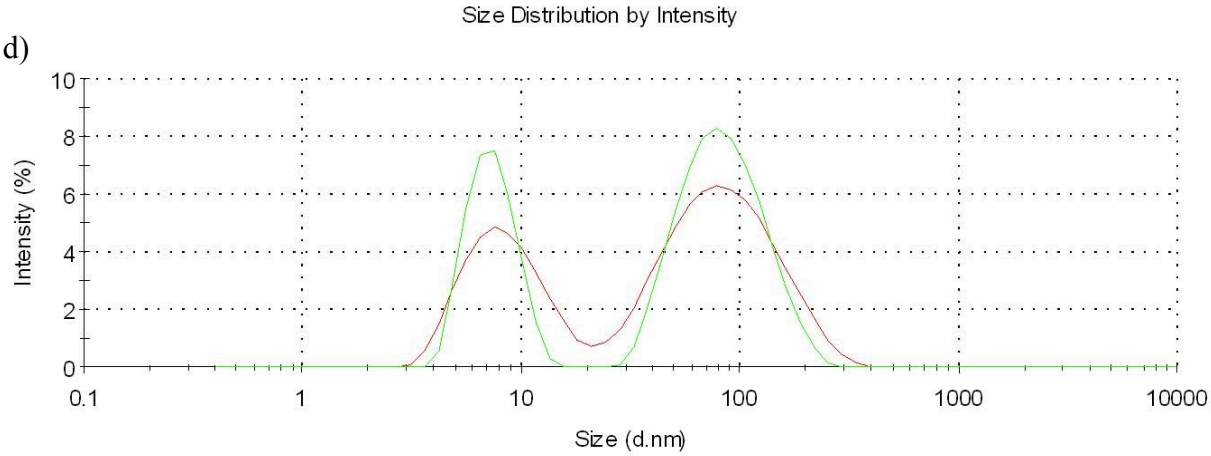


Figure S4. Correlation functions before (red) and after (green) addition of $JR2EC_2$ (b) and $JR2EC_{ref2}$ (b) and corresponding size distribution for $JR2EC_2$ (c) and $JR2EC_{ref2}$ (d).

References:

1. G. L. Ellman, *Arch. Biochem. Biophys.,* 1959, **82**, 70-77.

2. K. Enander, D. Aili, L. Baltzer, I. Lundström, B. Liedberg, *Langmuir* 2005, **21**, 2480-2487.

3. J.-J. Max, C. Chapados, *J. Phys. Chem. A*, 2004, **108**, 3324-3337.