## Supporting Information

## Thiol-free oligonucleotide surface modification of gold nanoparticles for nanostructure assembly

Anastasia Maslova, ${ }^{\text {a }}$ I-Ming Hsing ${ }^{*}{ }^{a}$
S1 - DNA sequences

| Name | Sequence |
| :--- | :--- |
| A1 | ATGACCATGTTATTACGAATTCGAGCTCGGTATTCCCGGGGATCCTCTAGAGTCGTTAGCTG <br> CAGCCAT |
| A2 | CGTATGTTGATCGACTCTAGAGGATCCCCGGGTTGCACTGGCCGTCGTGG <br> TACAATTCGTCGTGACTGG |
| A2-1 | CGTATGTTGATCGACTCTAGAGGATCCCCGGGTTGCACTGGCCGTCGTGGTACAATTCGTCG <br> TGACTGGCTTTCGTCCT |
| A2-1lc | CGTATGTTGATCGACTCTAGAGGATCCCCGGGTTGCACTGGCCGTCGTGGTACAATTCGTCG <br> TGACTGGAGGACGAAAG |
| A3 | TCCTGACGTTTTTGTACCACGACGGCCAGTGCTTACCCAACTTAATCGCCTTGCATTGCACA <br> TCCTTCG |
| A4 | CCAGCTGCCTTTGCAAGGCGATTAAGTTGGGTTTTACCGAGCTCGAATTCGTAATTTGTAAT <br> AGCGAAG |
| A4-I | CGAATTCGTAATTTGTAATAGCGAAGCCAGCTGGCTTTGCAAGGCGATTAAGTTGGGTTTTA <br> CCGAGCTCTTTCGTCCT |
| A4-IIc | CGAATTCGTAATTTGTAATAGCGAAGCCAGCTGGCTTTGCAAGGCGATTAAGTTGGGTTTTA <br> CCGAGCTAGGACGAAAG |
| B1 | CTTCGCTATTACTTTACGAGTTGTCGAATTGTTTGTTTAAAGTCTAATACTTCTACCTTTGG <br> CAGCTGG |
| B2 | CGAAGGATGTGCTTAGGTAGAAGTATTAGACTTTATTCTTCGCTATTACGCCAGCTGGTTAC <br> GACAGGA |
| B3 | CCAGTCACGACGTTCCAGCTGGCGTAATAGCGAAGTTCCTCAAATGTATTATCTATTGTTCA <br> ACATACG |
| B4 | ATGCGTGCAGCTTTCAATAGATAATACATTTGAGGTTCAAACAATTCGACAACTCGTATTCA <br> TGGTCAT |

Table S1. DNA sequences used for octahedron assembly.

Comment: ' or * sign shows complementarity (e.g. 11* region is complementary to 11 region), letters a and b correspond to 3 ' and 5 ' ends of DNA strands (see scheme below). Name xx-I and xx-IIc shows complementary


Figure S1. Default octahedron assembly with one ssDNA toehold.
toeholds for equal strands (for example, A2-I belongs to scaffold type 1 and hybridizes with A2-IIc of scaffold D2).

S2 - AFM image of control stock of encapsulated AuNPs in DNA cage.


S3 - AFM image of type 2 AuNPs


Figure S3. AFM image of type 2 AuNPs

S4 - Principal scheme of T2 type of AuNPs


Figure S4. T2 type octahedron.
S5 - AFM image of AuNPs pairs assembly


Figure S5. AFM image of AuNPs pairs assembly.

## S6 - HCR reaction

| Name | Sequence |
| :--- | :--- |
| Target | GCAGGAGTAGAAGATGGAGCAGC |
| Hp 1 | AAAAAAAAAAGCTGCTCCATCTTCTACTCCTGCATCCGGGCAGGAGTAGA <br> AGATGG |
| Hp2 | AAAAAAAAAAGCAGGAGTAGAAGATGGAGCAGCCCATCTTCTACTCCTGCCCGGAT |

DNA sequences for hairpins and a target:
Table S6. DNA sequences for HCR reaction: Hp 1 and Hp 2 stand for hairpin 1 and hairpin 2.


Figure S6. Lane 2: Control mixture of 2 hairpins without a target. Lanes 3-7: reaction mixture of 2 hairpins and the target in different molar ratio.

10\% PAGE gel for HCR products (without AuNPs):

## S7 - Polymerization

TEM images were taken of six samples with HCR reaction products. Number of chains were calculated (Table S3, Fig. S4):

| Length <br> (AuNPs) | Sample <br> 1 | Sample <br> 2 | Sample <br> 3 | Sample <br> 4 | Sample <br> 5 | Sample <br> 6 | Average <br> length | St. error |
| ---: | ---: | ---: | ---: | ---: | ---: | ---: | :--- | :--- |
| 1 | 50 | 38 | 40 | 32 | 56 | 25 | 40.16667 | 4.245368 |
| 2 | 27 | 12 | 11 | 12 | 9 | 8 | 13.16667 | 2.597185 |
| 3 | 4 | 3 | 9 | 5 | 4 | 5 | 5 | 0.781736 |
| 4 | 0 | 3 | 2 | 3 | 2 | 2 | 2 | 0.408248 |
| 5 | 2 | 1 | 1 | 0 | 2 | 0 | 1 | 0.333333 |
| 6 | 0 | 0 | 2 | 0 | 1 | 0 | 0.5 | 0.311805 |
| 7 | 1 | 1 | 0 | 2 | 0 | 0 | 0.666667 | 0.30429 |


| 8 | 0 | 0 | 1 | 0 | 0 | 0 | 0.166667 | 0.152145 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |



Figure S7. Chains length distribution based on Table S7.
Table S7. Number of chains with designated length in different samples.

