Electronic Supplementary Material (ESI) for Nanoscale
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Supporting Information

Protein-Nanoparticle Interactions: The effects of Surface Compositional and Structural Heterogeneity is Scale Dependent

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1. Particle size distribution of the three types of AuNPs used and the representative TEM image.

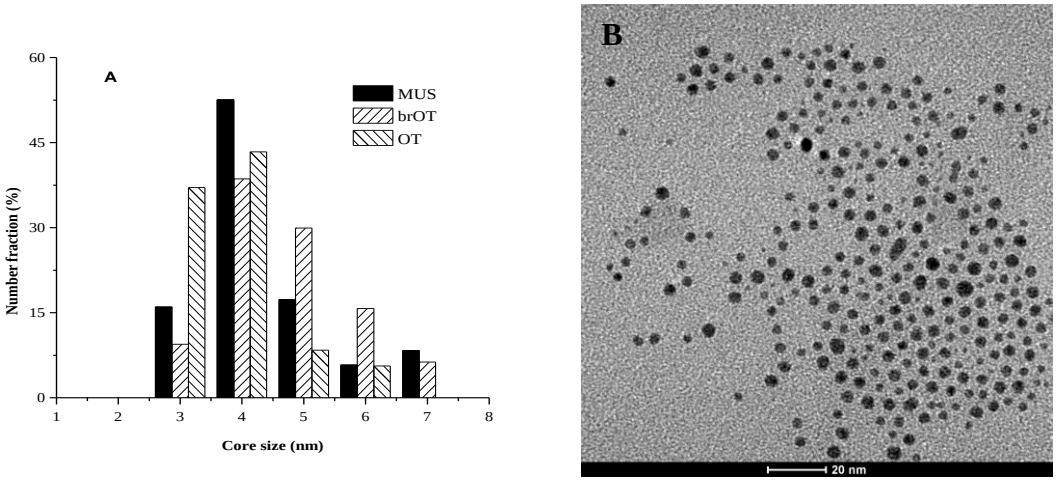

Figure S1. Size distribution of the three types AuNPs expressed in percentage (A) and a representative TEM image of the OT particles (B).

2. The titration of proteins into background buffer in the ITC experiment.

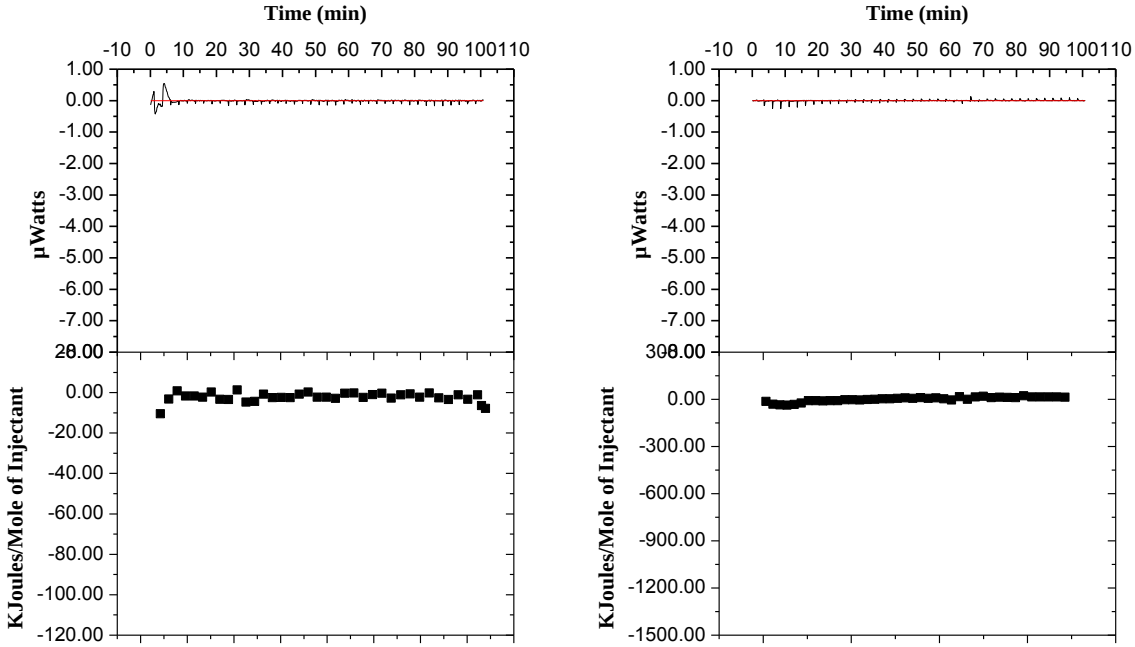

Figure S2. ITC data from the titration of 100 μM ubiquitin (left) and 80 uM fibrinogen (right) into 10 mM 7.4 phosphate buffer. Heat flow versus time during injection of proteins at 25 ℃ and heat evolved per injection of proteins was present above and below respectively.

3. The ITC results for ubiquitin interacting with 66-34 brOT and 66-34 OT AuNP.

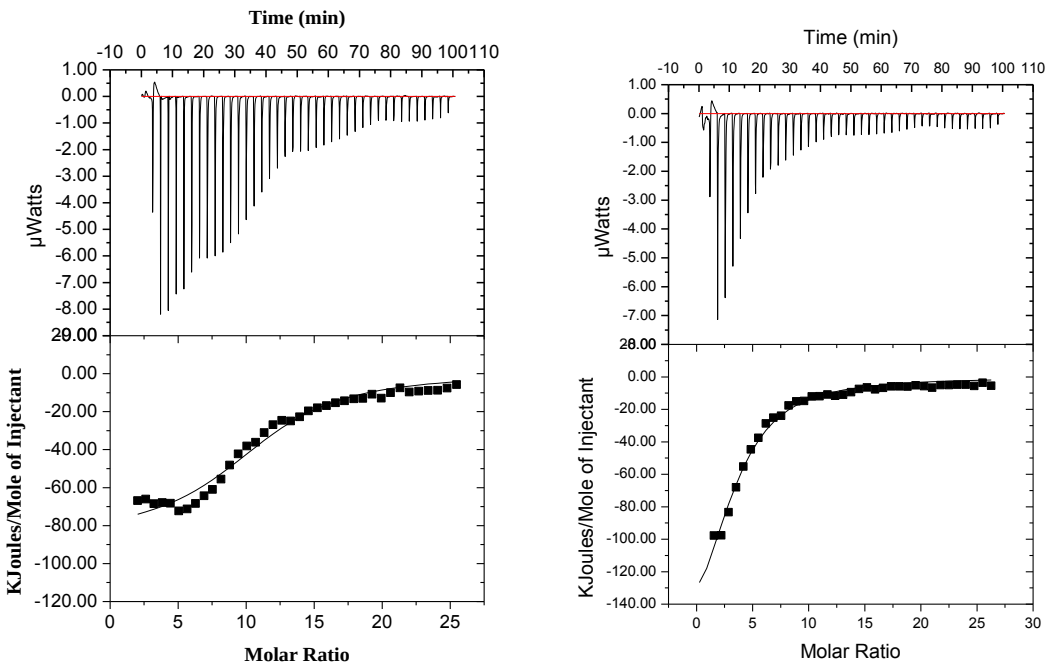

Figure S3. ITC data from the titration of 1 mM ubiquitin into 8.4 µM 66-34 brOT (left) and 7.7 µM 66-34 OT(right) AuNP. Heat flow versus time during injection of proteins at 25 ℃ and heat evolved per mole of added proteins (corrected for the heat of protein dilution) against the molar ratio (protein/AuNP) for each injection are shown at the top and bottom, respectively.

4. The ITC results for fibrinogen interacting with 66-34 brOT and 66-34 OT AuNP.

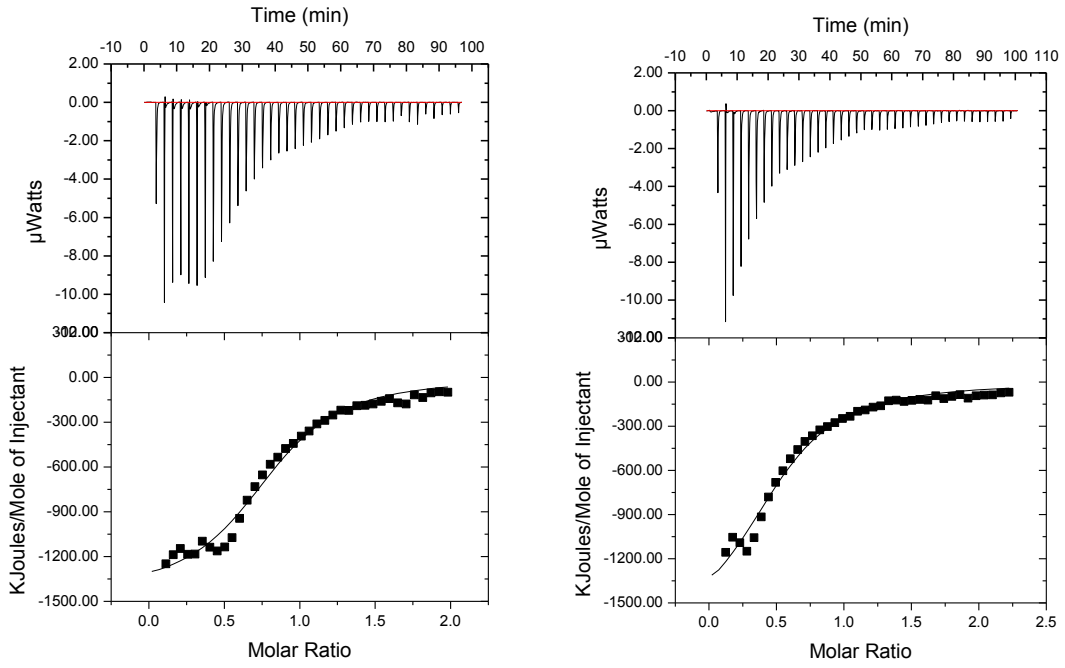

Figure S4. ITC data from the titration of 0.08 mM fibrinogen into 8.4 μM 66-34 brOT (left) and 7.7 μM 66-34 OT (right) AuNP. Heat flow versus time during injection of proteins at 25 ℃ and heat evolved per mole of added proteins (corrected for the heat of protein dilution) against the molar ratio (protein/AuNP) for each injection are shown at the top and bottom, respectively.

5. Determination of thermodynamic quantities by ITC.

Number concentration of the AuNPs was calculated from the mass concentration determined by ICP-MS with the Au core size characterized by TEM. The concentration of the proteins was determined based on the weight loaded into the solution. The concentration data were the only input needed by the Origin software coupled to the ITC to calculated the thermodynamic quantities, including binding stoichiometry. The heat change profiles were satisfactorily fit using a model describing a single set of binding sites. The parameters were calculated using nonlinear least-squares fitting.