Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Gold-Palladium core@shell nanoalloys: experiments and simulations

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$$\gamma = \frac{1}{2} - \frac{1}{2}\sin\left[\pi \frac{oe_i - oe_{mid}}{oe_{max} - oe_{min}}\right] \qquad oe_{mid} = \frac{oe_{min} + oe_{max}}{2}$$

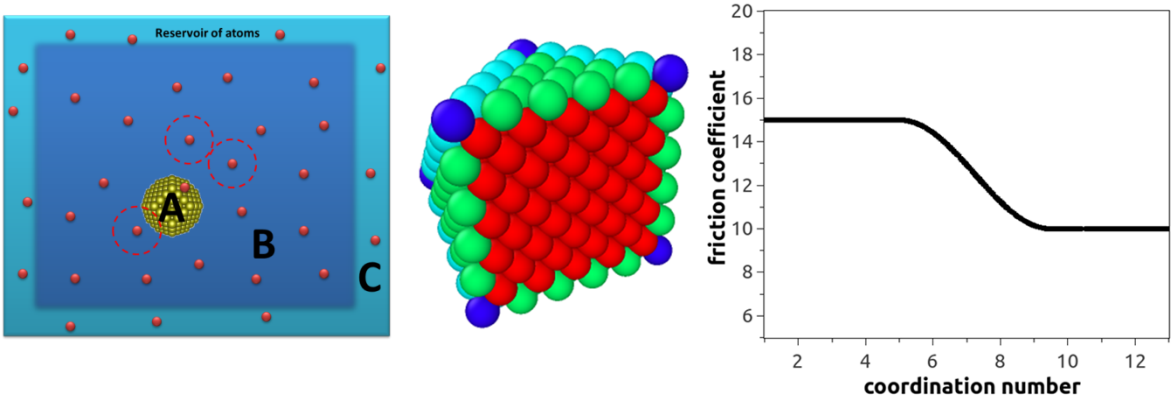

Figure S1: Left) GCLD model system: (A) cluster seed, (B) solution region and (C) reservoir of atoms. Right) cross-section of a typical nanoparticle where the atoms were colored according to its coordination number and dependence of the friction coefficient of each atom according to its coordination number.

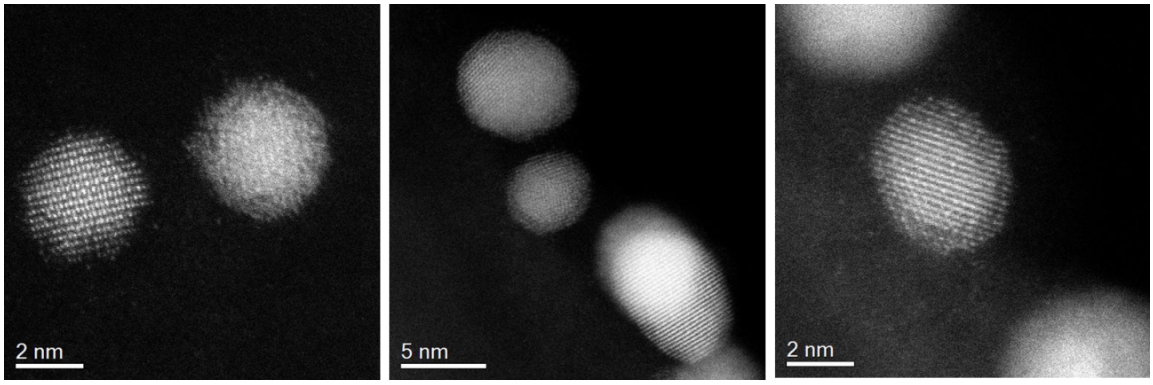

Figure S2: Diverse sub-5nm size core-shell NPs observed by Cs-STEM, in some of them, certain degree of mixing between Pd and Au is evident.

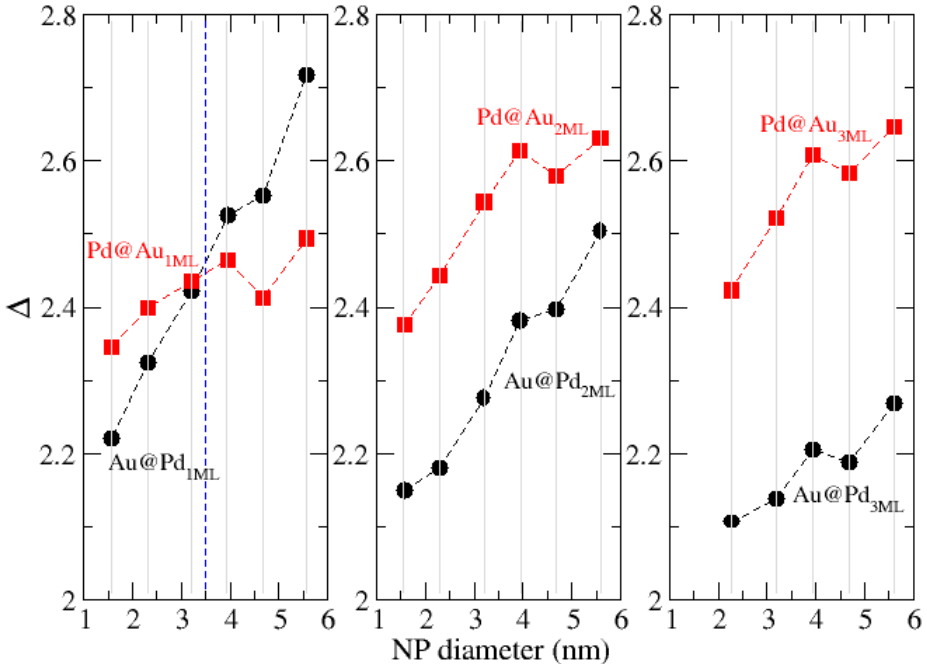

Figure S3: Excess energy as a function of NP size for core-shell with different shell-thickness (1 ML, 2 ML and 3 ML) for the case of Dh geometry.

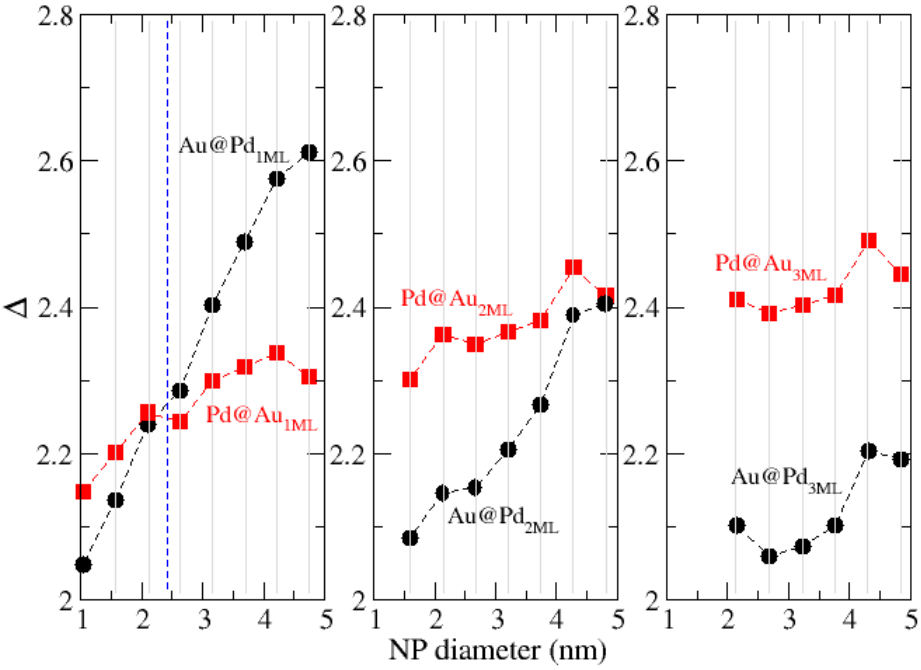

Figure S4: Excess energy as a function of NP size for core-shell with different shell-thickness (1 ML, 2 ML and 3 ML)for the case of Ih geometry

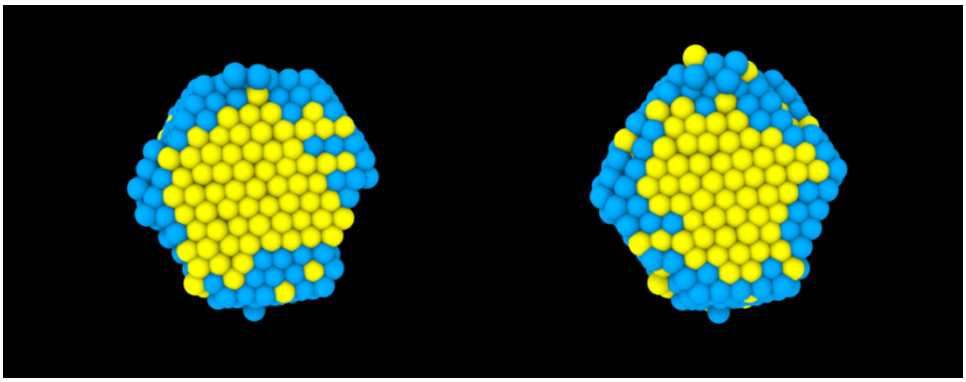

Figure S5: Cross-section images of figure 6f. Note the degree of mixing between Au and Pd in the interface region. Images produced with OVITO[1] software.

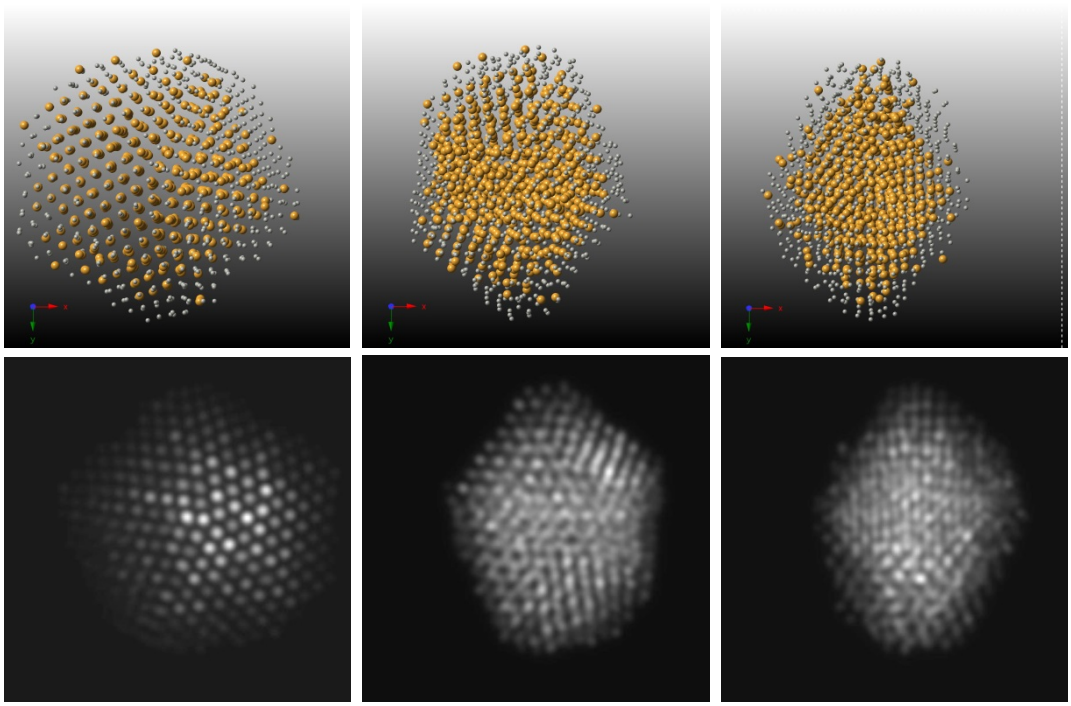

Figure S6: Simulated HAADF-STEM images of Dh Au(core)-Pd(shell) bimetallic nanoparticles at different orientations (left:0°, middle, 45° and right: 90°). Upper panel: configurations taken from gcLD, lower panel: HAADF-STEM simulations.

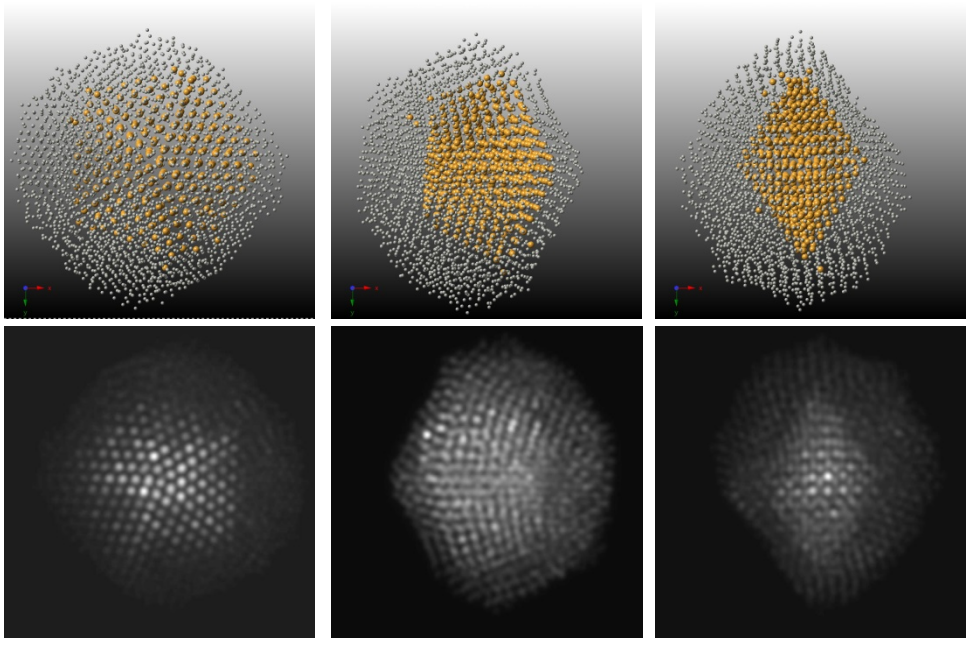

Figure S7: Simulated HAADF-STEM images of Dh Au(core)-Pd(shell) bimetallic nanoparticles at different orientations (left:0°, middle, 45° and right: 90°). Upper panel: configurations taken from gcMC, lower panel: HAADF-STEM simulations.

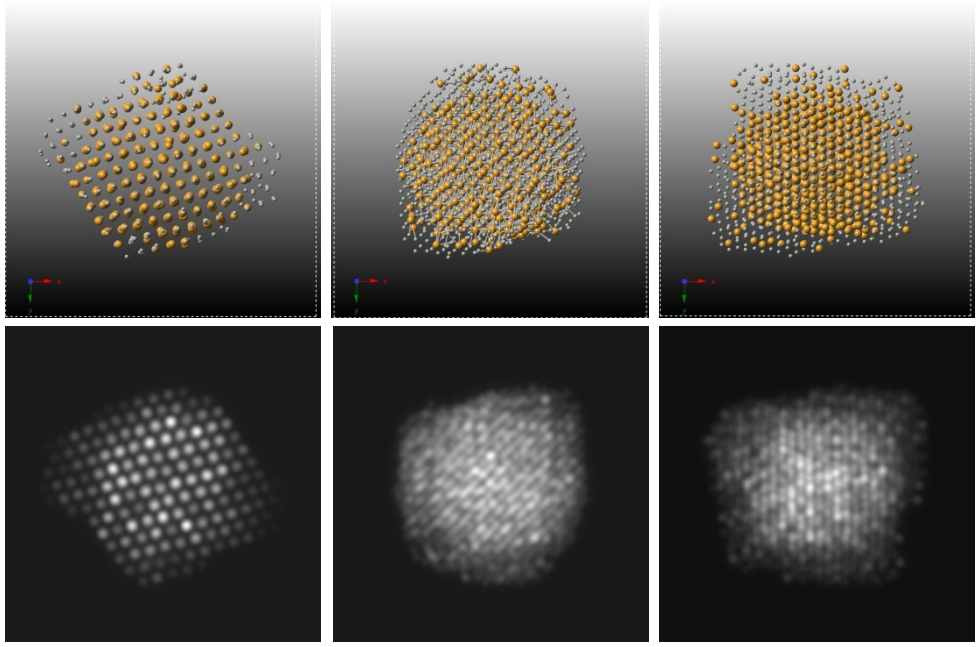

Figure S8: Simulated HAADF-STEM images of TOAu(core)-Pd(shell) bimetallic nanoparticles at different orientations (left:0°, middle, 45° and right: 90°). Upper panel: configurations taken from gcLD, lower panel: HAADF-STEM simulations.

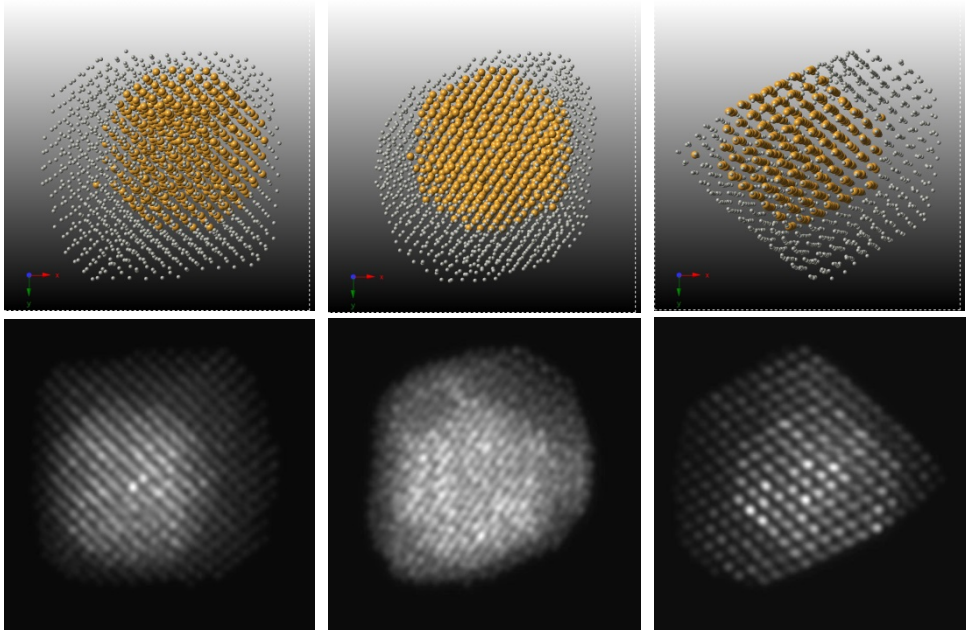

Figure S9: Simulated HAADF-STEM images of TO Au(core)-Pd(shell) bimetallic nanoparticles at different orientations (left: 0°, middle, 45° and right: 90°). Upper panel: configurations taken from gcMC, lower panel: HAADF-STEM simulations

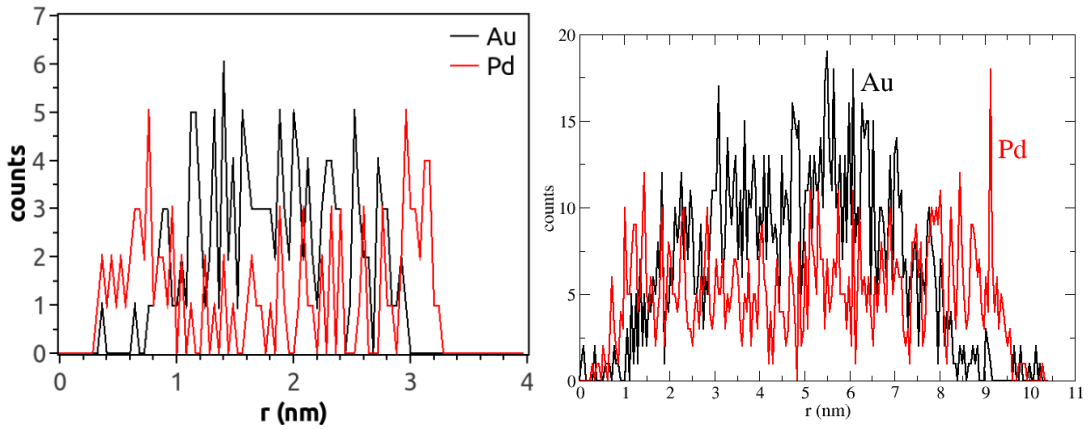

Figure S10: Left) Simulated EDS profile line of the resulting Dh Au(core)-Pd(shell) nanoparticles. Right) Experimental EDS profile line of a selected nanoparticle.

References:

1. A. Stukowski, *Simul. Mater.Sci. Eng.*2010, **18**, 015012.http://ovito.org