Supplementary Information

Gold-Palladium core@shell nanoalloys: experiments and simulations

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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.

\[ \gamma = \frac{1}{2} - \frac{1}{2} \sin \left[ \pi \frac{\text{OC}_{\text{min}} - \text{OC}_{\text{refl}}}{\text{OC}_{\text{min}} - \text{OC}_{\text{refl}}} \right] \quad \text{OC}_{\text{refl}} = \frac{\text{OC}_{\text{min}} + \text{OC}_{\text{max}}}{2} \]
**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\textsuperscript{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: