Supporting Information

Generalized nano-thermodynamic model for capturing size-dependent surface segregation in multi-metal alloy nanoparticles

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A. Equilibration with AgAuPd ternary alloy nanoparticle

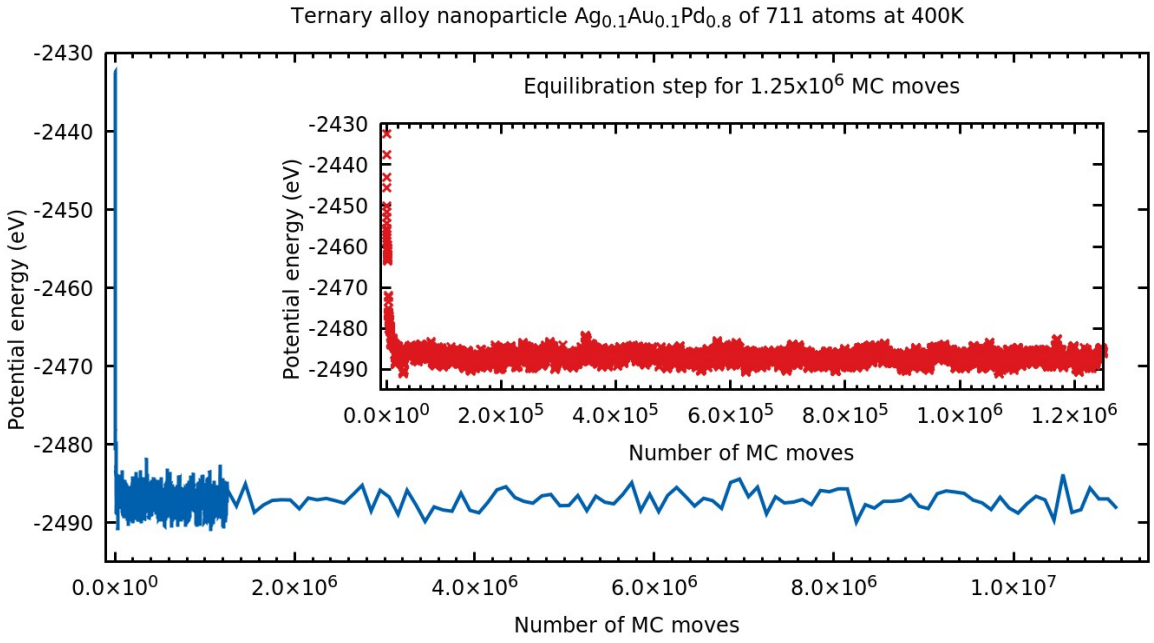

Fig. S1. The potential energy is plotted against the Monte Carlo steps for 711 atoms $Ag_{0.1}Au_{0.1}Pd_{0.8}$ nanoparticle for 11.25 million MC moves. The inset figure shows that the converged energy is attained well before 1 million steps.

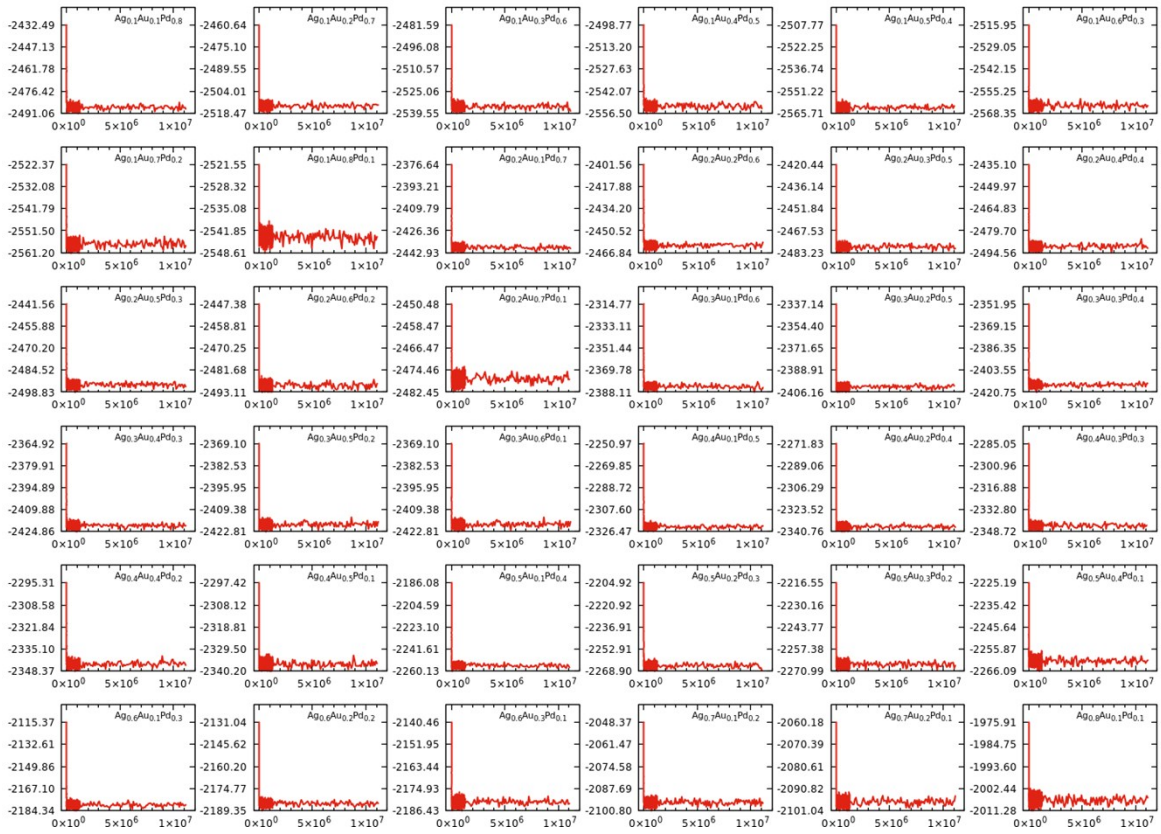

Fig. S2. The potential energy is plotted against the Monte Carlo steps for 711 atoms of 36 Ag-Au-Pd nanoparticles for 11.25 million MC moves.

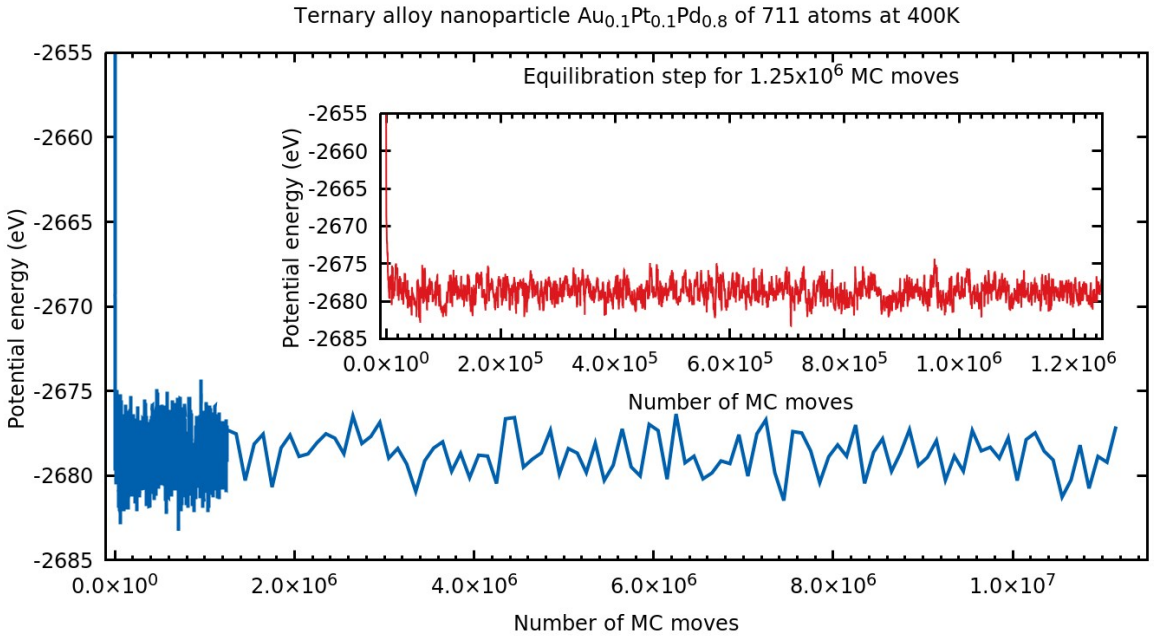

Fig. S3. The potential energy is plotted against the Monte Carlo steps for 711 atoms $Au_{0.1}Pt_{0.1}Pd_{0.8}$ nanoparticle for 11.25 million MC moves. The inset figure shows that the energy is well converged before 1 million steps.

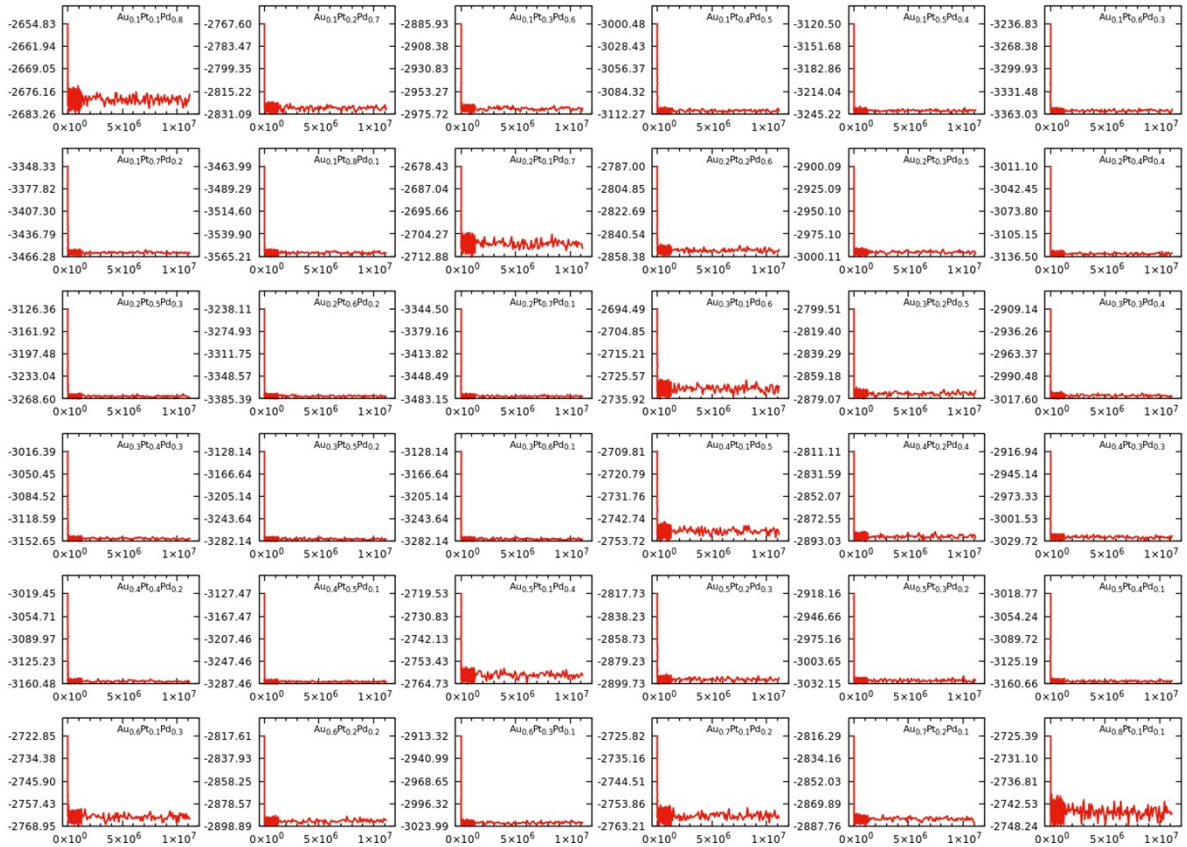

Fig. S4. The potential energy is plotted against the Monte Carlo steps for 711 atoms of 36 AuPtPd nanoparticles for 11.25 million MC moves.

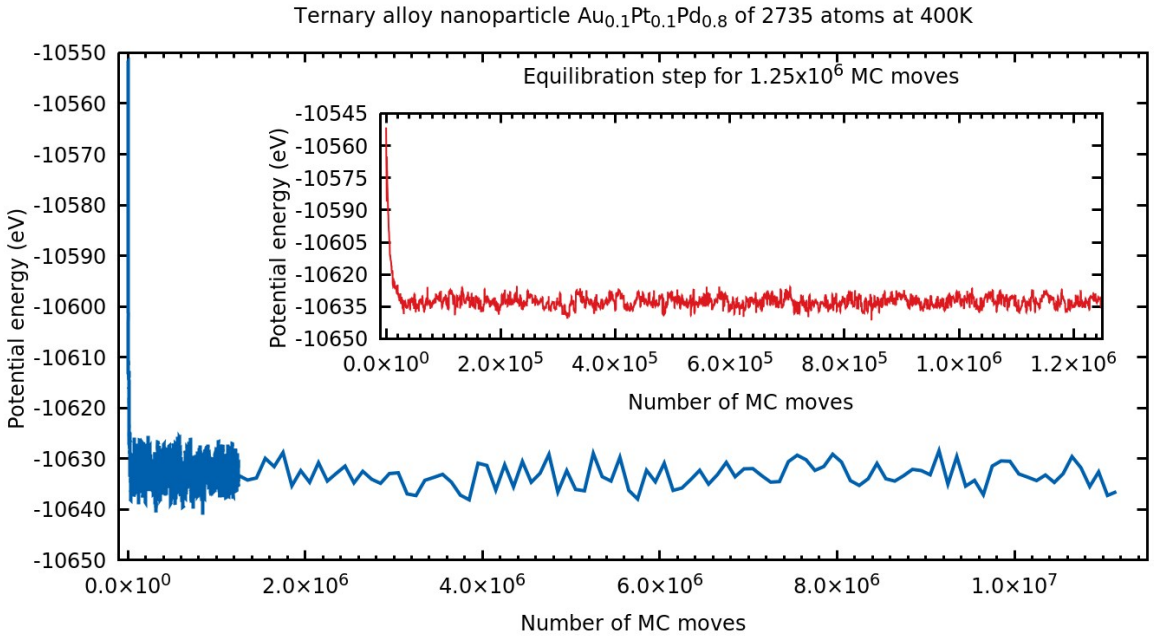

Fig. S5. The potential energy is plotted against the Monte Carlo steps for 2735 atoms $Au_{0.1}Pt_{0.1}Pd_{0.8}$ nanoparticle for 11.25 million MC moves. The inset figure shows that the energy is well converged before 1 million steps.

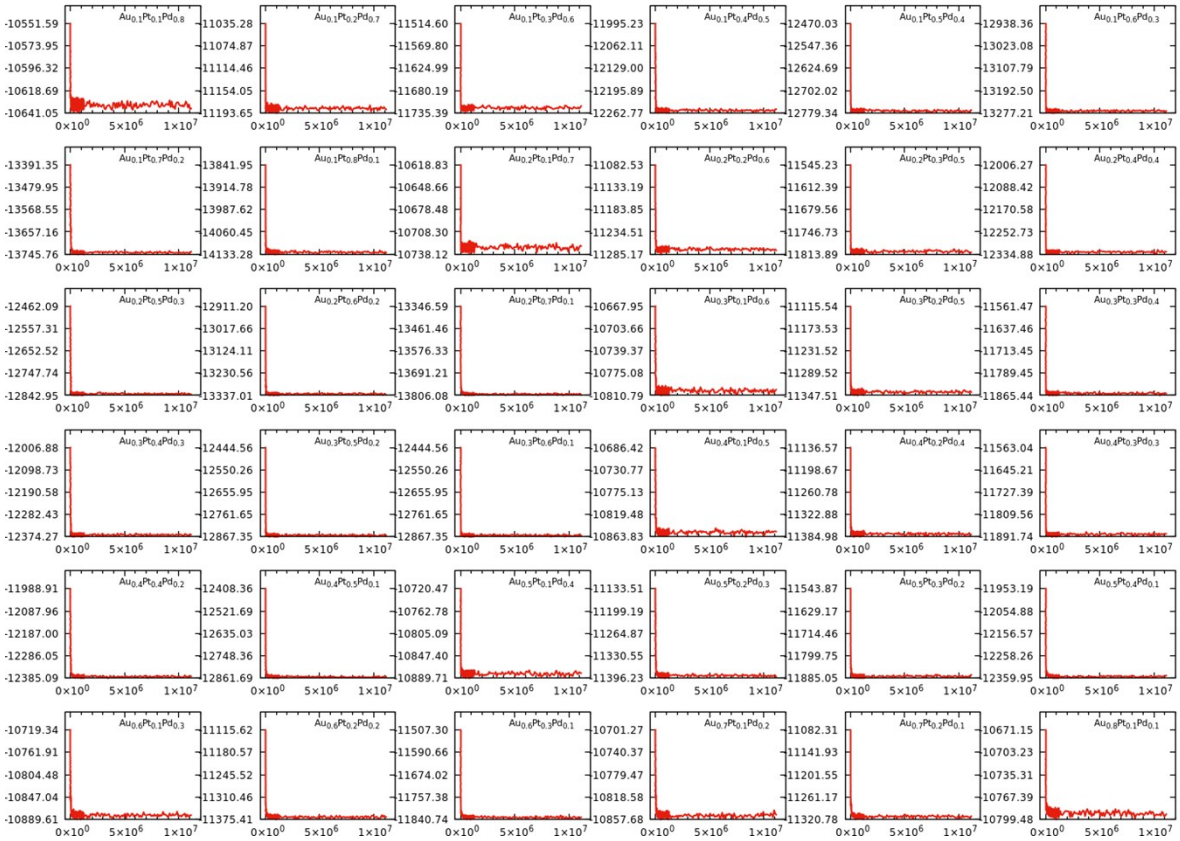

Fig. S6. The potential energy is plotted against the Monte Carlo steps for 2735 atoms of 36 AuPtPd nanoparticles for 11.25 million MC moves.

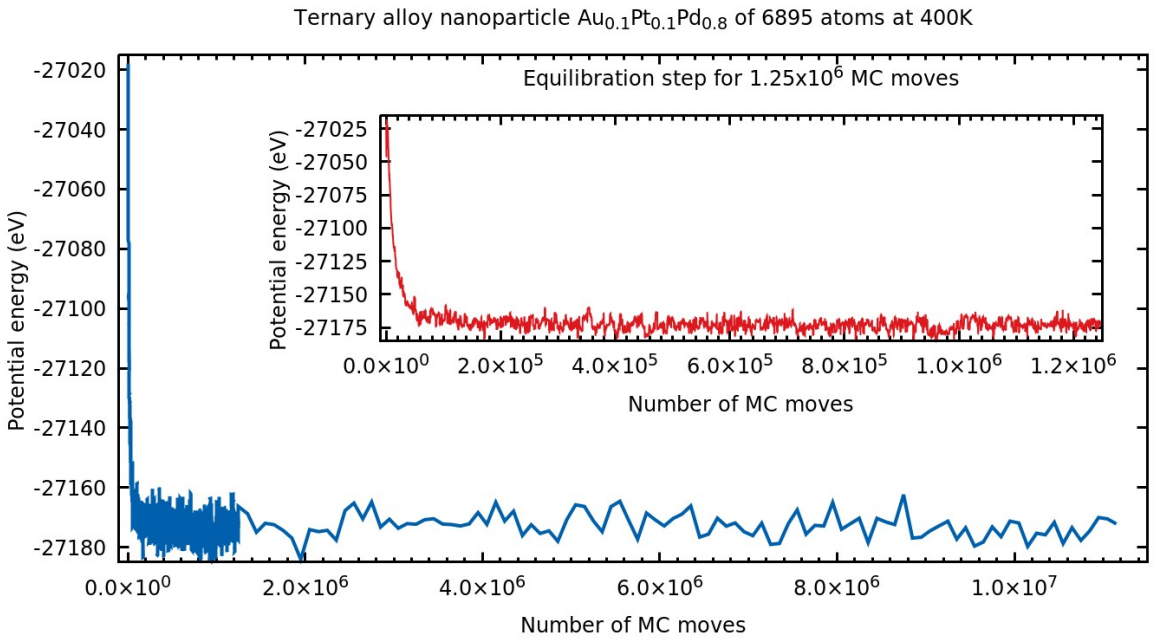

Fig. S7. The potential energy is plotted against the Monte Carlo steps for 6895 atoms $Au_{0.1}Pt_{0.1}Pd_{0.8}$ nanoparticle for 11.25 million MC moves. The inset figure shows that the energy is well converged before 1 million steps.

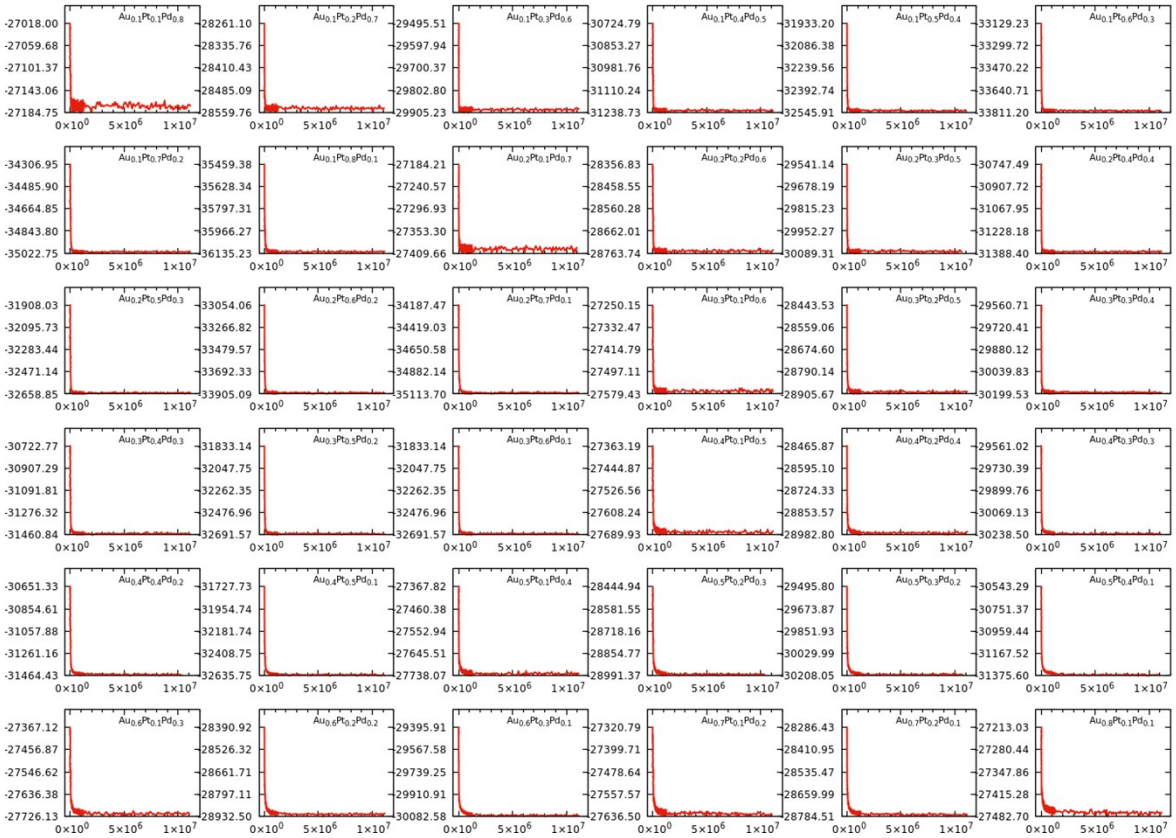

Fig. S8. The potential energy is plotted against the Monte Carlo steps for 6895 atoms of 36 AuPtPd nanoparticles for 11.25 million MC moves.

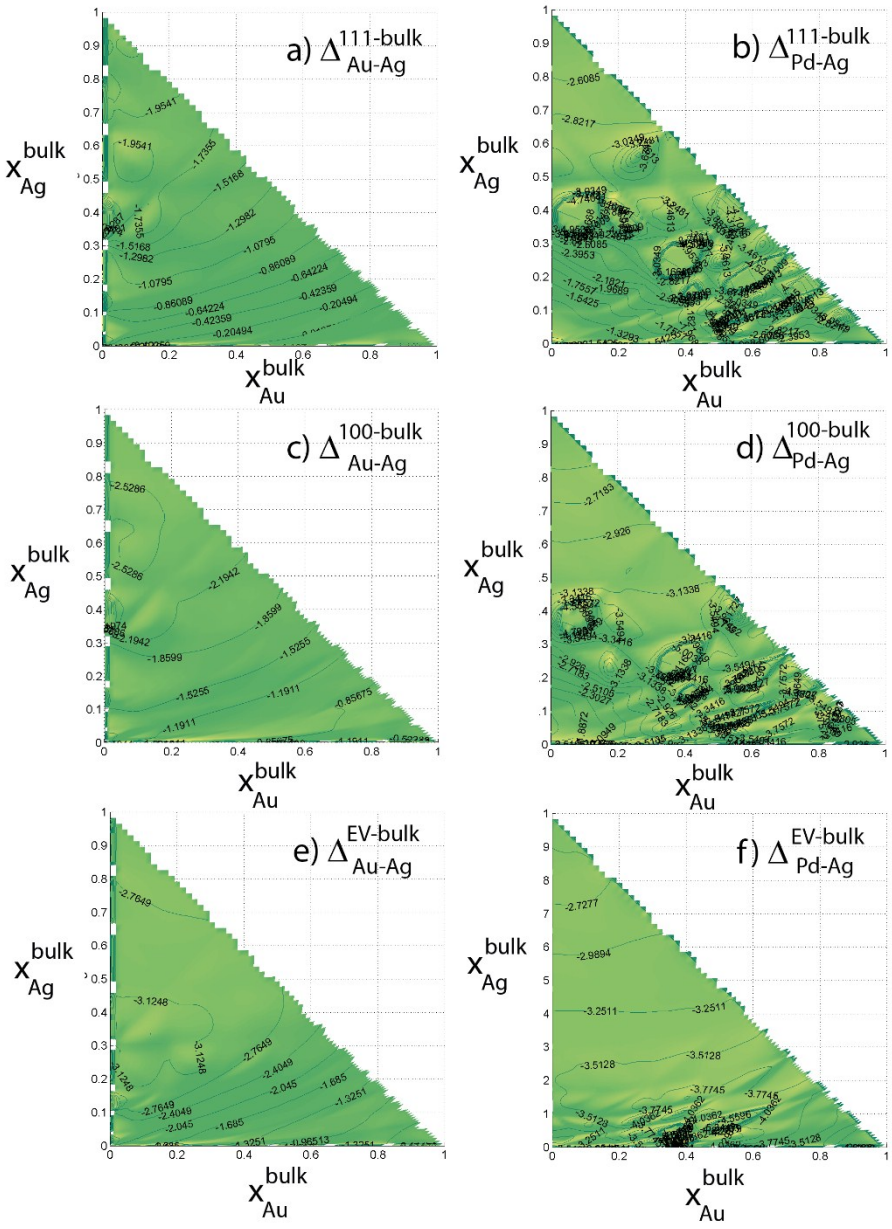

Fig. S9. Distribution coefficients for 711 atom Ag-Au-Pd NP (in $\log_{10}$) as a function of the Au and Ag composition of the bulk.

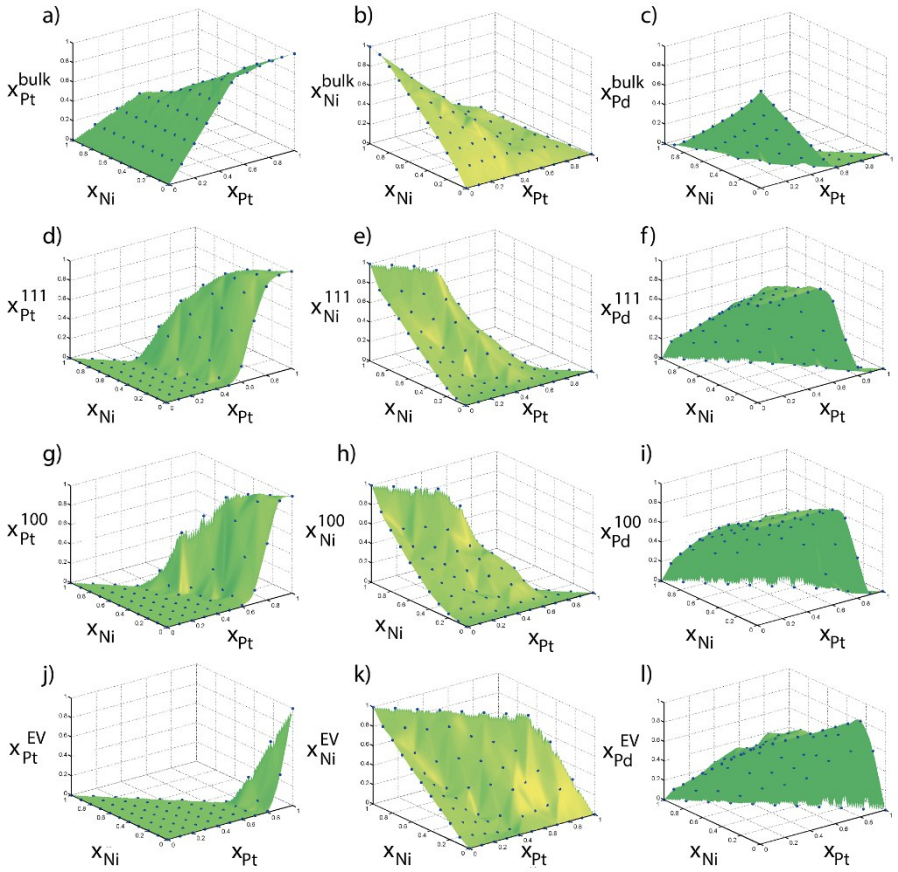

Fig. S10. Compositions measured using Monte Carlo simulations for 711 atom Ni-Pt-Pd NP are shown in points. Surface was generated using Delaunay triangulation of the data.

Table S1: Size of the periodic box in Å used for the Monte Carlo calculations

NP size	x	y	z
711 atoms	43.15	44.16	40.66
2735 atoms	75.12	75.12	93.9
6895 atoms	97.53	97.53	116.15