# Electronic Supplementary Information

**Magnetism in Bimetallic $Pt_xNi_{N-x}$ Clusters via Cross-Atomic Coupling**

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## Equilibrium Structures

The interaction between metal atoms was modeled semi-empirically based on the well-established Gupta potential. The explicit form of the Gupta potential can be expressed as

$$E_{total} = \sum_{i}^{N}\left(\sum_{j\neq i}^{N} Ae^{-p\left(r_{ij}/r_0-1\right)} - \sqrt{\sum_{j\neq i}^{N}\xi^2 e^{-2q\left(r_{ij}/r_0-1\right)}}\right) \qquad \text{(S1)}$$

where, $r_{ij}$ is the distance between atoms $i$ and $j$ in the cluster, $r_0$ is the nearest-neighbor distance in the pure metal, and $N$ is the number of the metal atoms. The parameters ($A$, $\xi$, $p$, $q$) of the potential for the $Pt_xNi_{N-x}$ clusters used in this work are

taken from the literature and shown in Electronic Supplementary Information (ESI) Table S1.[1, 2] The semi-grand-canonical (Δμ, *NPT*) ensemble Monte Carlo (SEMI-GCMC) simulation was undertaken to obtain the initial equilibrium structures of the bimetallic $Pt_xNi_{N-x}$ clusters. More details of the SEMI-GCMC method was documented in our previous works, and was found to be effective to obtain the initial equilibrium structures of $Pt_xNi_{N-x}$ clusters.[2] Here, like in our previous simulation, two trials are introduced in the Monte Carlo sampling scheme: (1) Random displacement of one atom from its original position, and (2) random interchange of two atoms with different species. During the equilibrium stage (depends on temperature, typically after 500,000 MC steps), detailed balance is observed with relatively small fluctuation in total energy, as shown in ESI Fig. S5.

As mentioned above, here we focus on the $Pt_xNi_{N-x}$ ($N$ = 13, 55, 147) clusters with of CUBO, DEC, and ICO morphologies, and all with one of the four distinct chemical orders structures, including (1) the core-shell structure, in which Pt atoms segregate at the surface and Ni atoms are in the core; (2) onion-ring structure, in which the Pt atoms are located on the surface and the Ni atoms are in the subsurface shell, then Pt and Ni shells take turn alternatively; (3) layer structure ($L1_0$-ordered), in which single layer of Ni and Pt is stacked alternatively in the [001] direction;[3] and (4) crown structure, in which 12 Ni atoms occupy the vertex sites on the surface layer. Note that for disordered icosahedral or poly-icosahedral structure, the equilibrium structure has a Ni rich region after conducting SEMI-GCMC simulation. So, for the ordered (core-shell, onion-ring, L10-orderd and crown) icosahedral or poly-icosahedral structures, the equilibrium structure are obtained by artificial modeling, then all the initial structures are re-optimized by using first-principles density functional theory (DFT) methods.

**Effect of single impurity Ni on the magnetic properties of the PtNi alloying clusters.**

Adding magnetic 3d Ni atoms into the Pt clusters will undoubtedly result in richer magnetic properties for the PtNi alloying clusters. The computed magnetic properties of $Pt_{N-1}Ni_1$ ($N$ = 13, 55, 147) clusters with either cuboctahedron (CUBO), decahedron (DEC), or icosahedron (ICO) morphology are shown in Fig. S6. Fig. S6(a) shows that

the magnetic moments of $Pt_{N-1}Ni_1$ clusters with CUBO, EDC, and ICO morphology decrease as $N$ increases: $Pt_{12}Ni_1$ cluster exhibits the highest magnetic moment (3.98μB), followed by that (3.96μB) of $Pt_{54}Ni_1$. $Pt_{146}Ni_1$ cluster possesses the lowest magnetic moments (0.18μB) among the three sizes. The same trend holds for the $Pt_{N-1}Ni_1$ clusters with DEC and ICO morphologies. From $Pt_{12}Ni_1$ to $Pt_{146}Ni_1$, the magnetic moments are $3.80\mu_B$, $3.72\mu_B$, and $0.18\mu_B$ with DEC morphology, and are $3.44\mu_B$, $3.41\mu_B$, and $0.07\mu_B$ with ICO morphology. Hence, the size can greatly affect the magnetic properties of small- to mid-sized $Pt_{N-1}Ni_1$ clusters. Moreover, comparing the magnetic properties of $Pt_{N-1}Ni_1$ clusters with different morphology but the same size, we find that the morphology has little influence on the magnetic moment.

**Table S1.** Computed total magnetization ($\mu_B$) for $Pt_xNi_{55-x}$ clusters with cuboctahedron (CUBO), decahedron (DEC), and icosahedron (ICO) morphologies, respectively.

| Composition of | morphologies | | |
|---|---|---|---|
| Pt | CUBO | ICO | DEC |
| 0 | 40.11 | 40.07 | 40.04 |
| 0.1 | 39.91 | 40.30 | 39.76 |
| 0.2 | 38.30 | 39.46 | 36.99 |
| 0.3 | 39.35 | 38.78 | 36.74 |
| 0.4 | 37.55 | 36.97 | 35.85 |
| 0.5 | 36.86 | 35.54 | 33.53 |
| 0.6 | 32.50 | 31.20 | 31.57 |
| 0.7 | 23.64 | 23.58 | 25.08 |
| 0.8 | 21.27 | 22.03 | 22.69 |
| 0.9 | 10.18 | 14.68 | 15.52 |
| 1.0 | 0.16 | 0.06 | 0.23 |

**Table S2.** The fitted parameters of the TB-SMA potential for PtNi nanoparticles.

| | A (eV) | $\xi$ | p | q |
|---|---|---|---|---|
| Pt-Pt | 0.1602 | 2.1855 | 13.00 | 3.13 |
| Ni-Ni | 0.0845 | 1.405 | 11.73 | 1.93 |
| Pt-Ni | 0.1346 | 2.3338 | 14.838 | 3.036 |

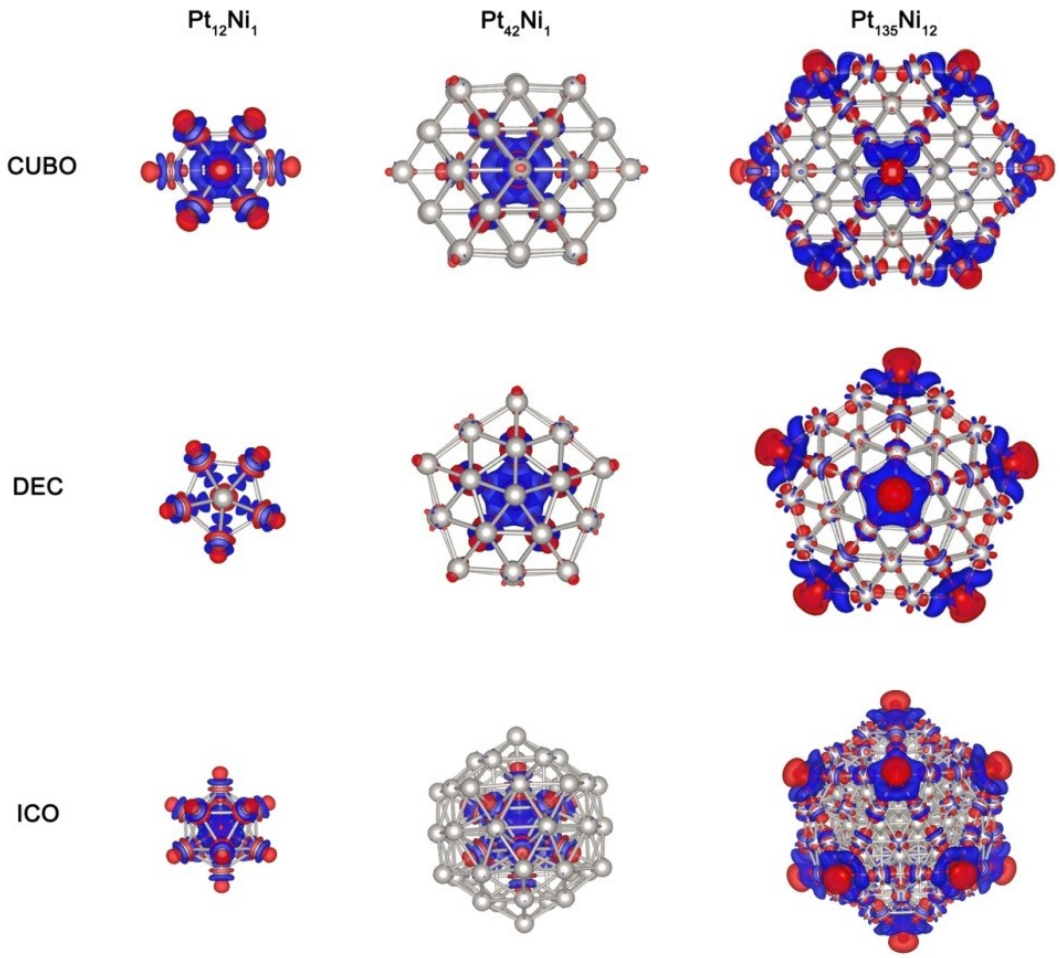


**Fig. S1.** Computed charge density difference of $Pt_{12}Ni_1$, $Pt_{44}Ni_1$ and $Pt_{135}Ni_{12}$ clusters with the core-shell order and one of three possible morphologies CUBO (top), DEC (middle), and ICO (bottom).

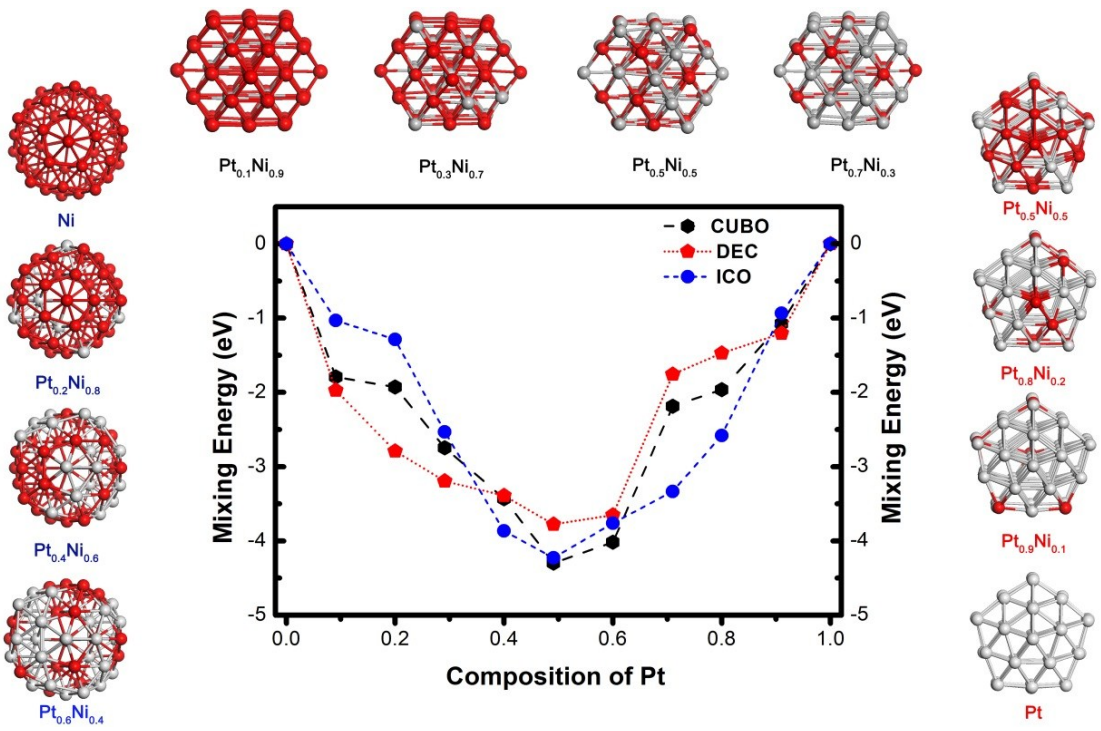


**Fig. S2.** Computed mixing energies of $Pt_xNi_{N-x}$ ($N$ = 55) clusters with cuboctahedron (CUBO), decahedron (DEC), or icosahedron (ICO) morphologies *versus* the Pt composition.

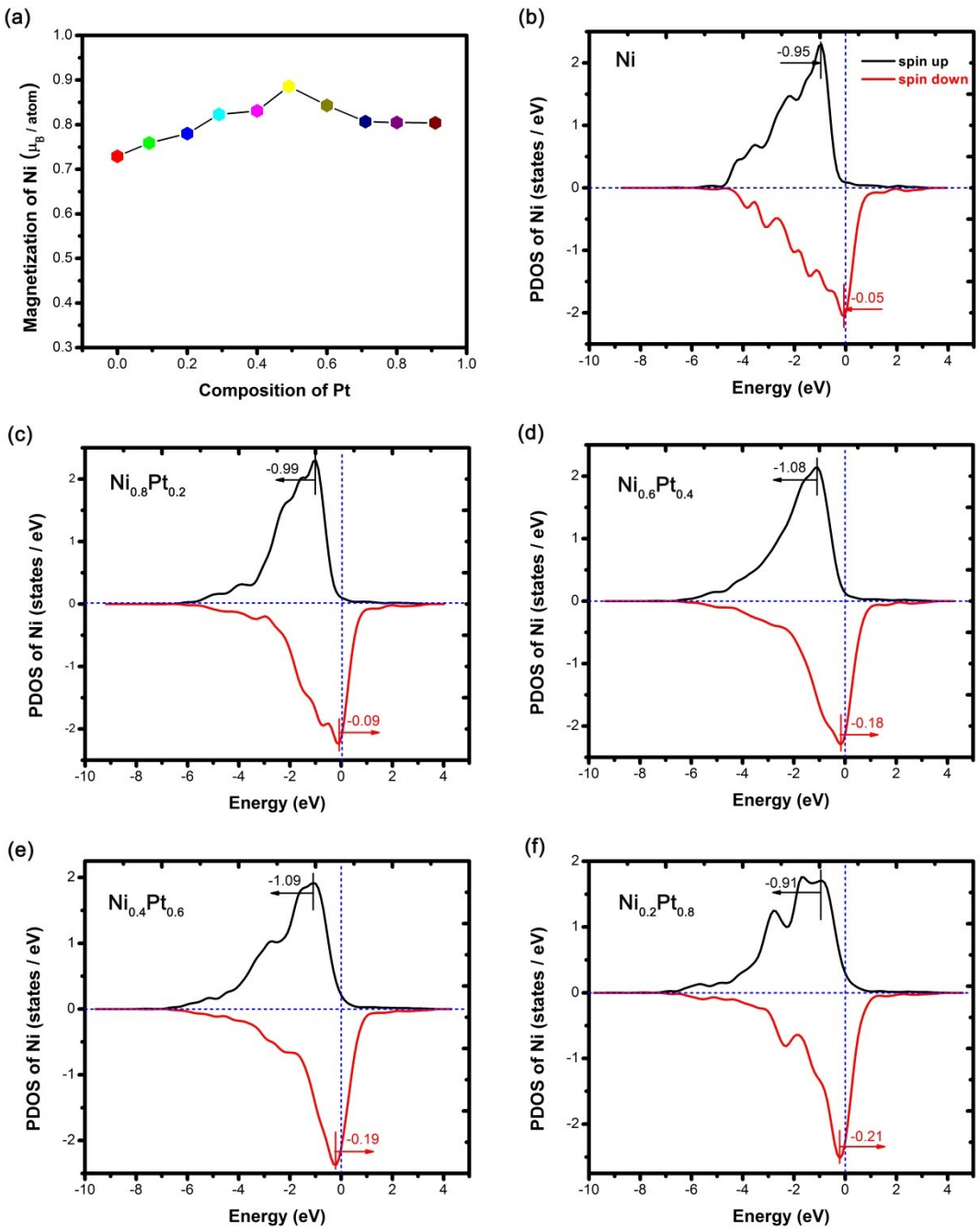


**Fig. S3.** (a) Computed magnetization of Ni atom in $Pt_xNi_{N-x}$ ($N$ = 55) clusters with different Pt composition; (b-f) computed PDOS of the *d* orbital of Ni *versus* the Pt composition (the concentration of Pt increases with step of 20%). The Fermi level is denoted by a vertical dashed line at zero.

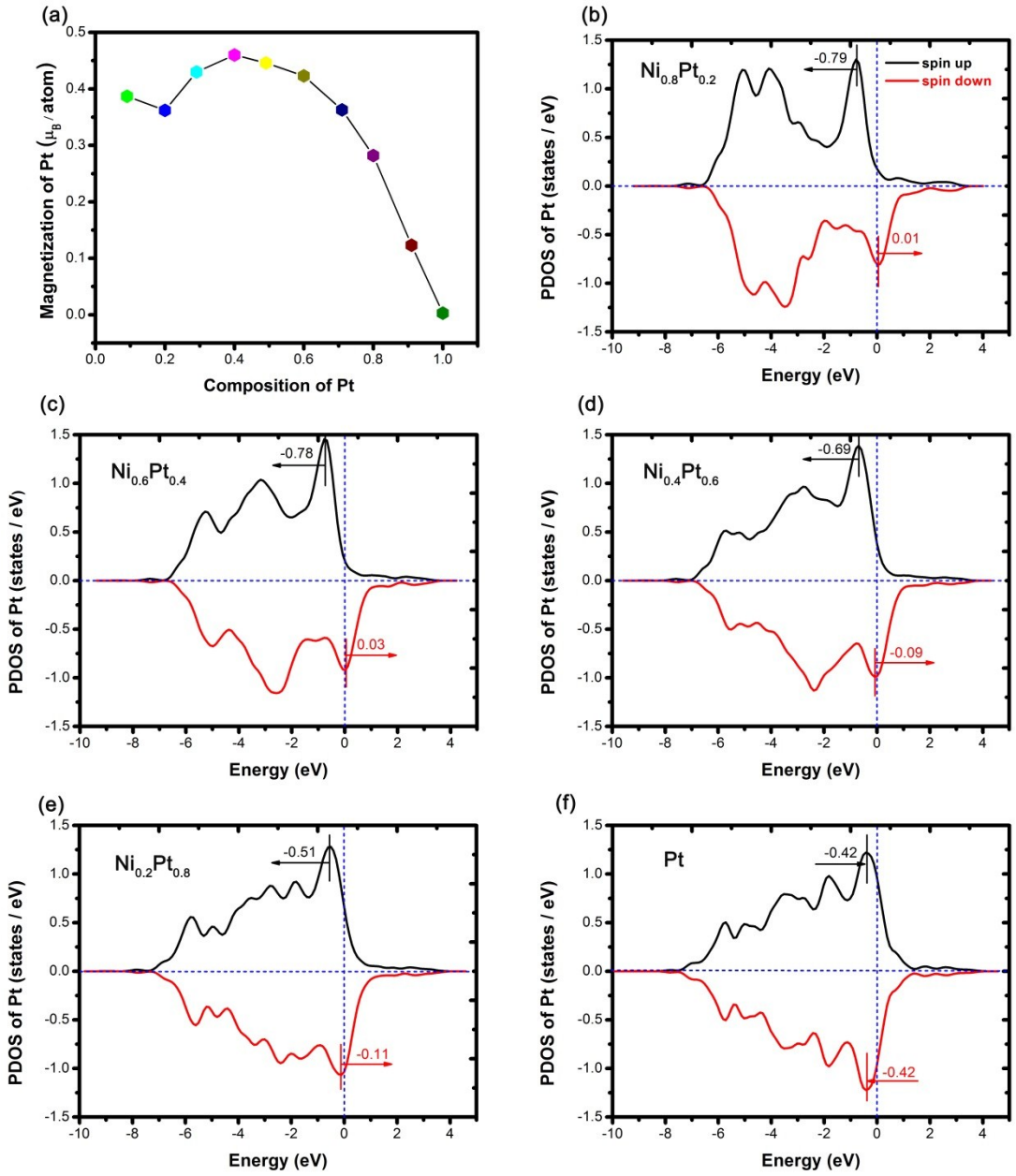


**Fig. S4.** (a) Computed the magnetization of the Pt atom in $Pt_xNi_{N-x}$ ($N$ = 55) clusters with different Pt composition; (b-f) computed PDOS of the *d* orbital of Pt versus the Pt composition (the concentration of Pt increases with step of 20%). The Fermi level is denoted by a vertical dashed line at zero.

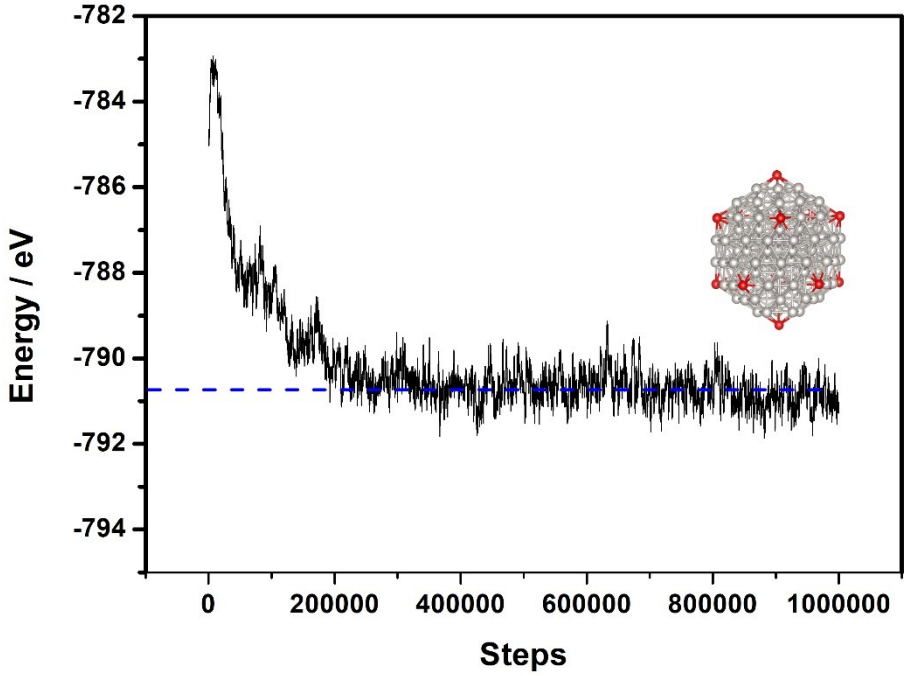


**Fig. S5.** Monte Carlo (MC) simulation for $Pt_{135}Ni_{12}$ cluster with the crown order and ICO morphology. After 500000 MC steps, the structure is in equilibrium stage.

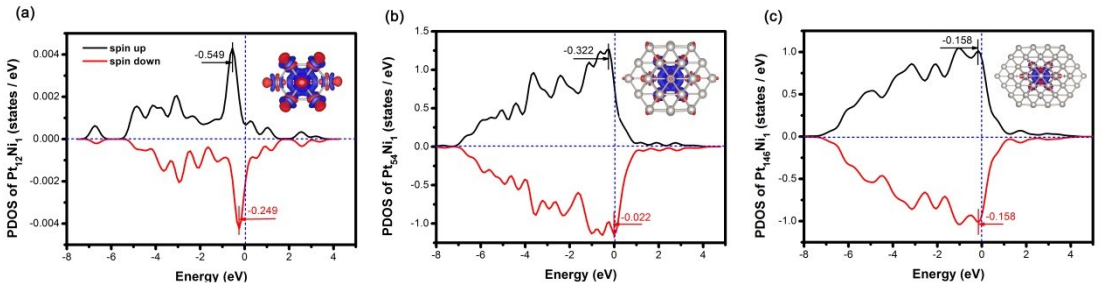


**Fig. S6.** Computed PDOS of the *d*-orbital; charge-density difference of $Pt_{12}Ni_1$, $Pt_{54}Ni_1$, and $Pt_{146}Ni_1$ clusters with the cuboctahedron morphology being shown in insets.

We list the coordinates of the 147- atom pure Pt cluster with cuboctahedron (CUBO), decahedron (DEC), and icosahedron (ICO) morphologies in ESI. All the initial structure of PtNi alloy clusters with different composition, ordering (core-shell, onion-ring, L10-orderd and crown), and size (<147) can be obtained from the structure of the 147- atom pure Pt cluster.

ICO /147

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DEC/147

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| Pt | 9.965400000 | 12.370000000 | 4.731000000 |
| Pt | 11.918200000 | 10.446600000 | 4.815200000 |

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