Supplementary Materials

First-Principles Investigation of Size Effects on Cohesive Energies of Transition-Metal Nanoparticles

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**Table 1.** List of Parameters '*a*' and '*b*' in the Natural Logarithmic Function for Fitting Cohesive Energies of Nanoparticles. .

|  |  |  |
| --- | --- | --- |
| **Element**  | ***a***  | ***b***  |
| Sc  | 0.72504841  | 2.20934348  |
| Ti  | 0.89810472  | 12.01789744  |
| V  | 1.16951657  | 1.02238005  |
| Cr  | 0.79397321  | 0.48902491  |
| Mn  | 0.61779602  | 1.1861684  |
| Fe  | 0.80001186  | 3.91109861  |
| Co  | 0.824159  | 4.70718674  |
| Ni  | 0.72964512  | 4.99065518  |
| Cu  | 0.55160499  | 4.20072647  |
| Zn  | 0.1913661  | 0.55464114  |
| Y  | 0.75614744  | 5.3667668  |
| Zr  | 1.00990119  | 4.09499696  |
| Nb  | 1.04150976  | 6.20878157  |
| Mo  | 1.35036784  | 0.96117769  |
| Tc  | 1.11531218  | 3.74701285  |
| Ru  | 1.01494177  | 4.02485467  |
| Rh  | 0.83450127  | 5.01848205  |
| Pd  | 0.58276816  | 3.03765054  |
| Ag  | 0.42541707  | 3.13586064  |
| Cd  | 0.11033387  | 0.67963352  |
| La  | 0.71446756  | 6.1480644  |
| Hf  | 1.21114911  | 6.83491705  |
| Ta  | 1.18925133  | 6.83612842  |
| W  | 1.17388636  | 5.396755  |
| Re  | 1.37633963  | 2.12208248  |
| Os  | 1.30260075  | 3.99292611  |
| Ir  | 1.02817762  | 7.76355096  |
| Pt  | 0.76148922  | 9.64927626  |
| Au  | 0.48851975  | 4.77290778  |
| Hg  | 0.02775863  | 1.30970181  |



**Figure 1.** Calculated cohesive energy per atom as a function of the nanoparticle size (*n*) for transition-metal nanoparticles (X*n*) in period 4 (a) X = Sc, (b) X = Ti, (c) X = V, (d) X = Cr, (e) X.= Mn, (f) X = Fe.

 

**Figure 2.** Calculated cohesive energy per atom as a function of the nanoparticle size (n) for transition-metal nanoparticles (Xn) in period 4 (a) X = Co, (b) X = Ni, (c) X = Cu, (d) X = Zn.



**Figure 3.** Calculated cohesive energy per atom as a function of the nanoparticle size (*n*) for transition-metal nanoparticles (Xn) in period 5 (a) X = Y, (b) X = Zr, (c) X = Nb, (d) X = Mo, (e).X = Tc, (f) X = Ru.



**Figure 4.** Calculated cohesive energy per atom as a function of the nanoparticle size (*n*) for transition-metal nanoparticles (X*n*) in period 5 (a) X = Rh, (b) X = Pd, (c) X = Ag, (d) X = Cd.



**Figure 5.** Calculated cohesive energy per atom as a function of the nanoparticle size (*n*) for transition-metal nanoparticles (X*n*) in period 6 (a) X = La, (b) X = Hf, (c) X = Ta, (d) X = W, (e) X = Re, (f) X = Os.



**Figure 6.** Calculated cohesive energy per atom as a function of the nanoparticle size (*n*) for transition-metal nanoparticles (X*n*) in period 6 (a) X = Ir, (b) X = Pt, (c) X = Au, (d) X = Hg.



**Figure 7.** Heat map illustrating (a) the calculated cohesive energy (eV/atom) for transition-metal nanoparticles X4 and (b) the experimental values of the transition-metal bulk structures.