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. .

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| --- | --- | --- |
| **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 |

A collage of graphs

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**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.

A group of graphs with different colored dots

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**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.

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**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.

A group of graphs with different colored dots

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**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.

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**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.

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**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.

A table of periodic table of elements

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**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.