# Supplementary Material for

Machine-Learning-Augmented Chemisorption Model for $CO_2$ Electroreduction Catalyst Screening

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## 1. Computational Details

Electronic structure calculations were performed within the framework of spin-polarized density functional theory (DFT) implemented in Quantum ESPRESSO[1] using Perdew-Burke-Ernzerh (PBE) exchange-correlation functional.[2] The {100}-terminated surfaces were modelled by a four-layer slab for bimetallics and a 5-layers slab for multimetallics with 4×2 supercells and 15 Å of vacuum space. The adsorbates and the two topmost metal layers were fully relaxed until the forces were smaller than 0.05 eV/Å while other metal layers were held fixed in their bulk positions. The Brillouin zones of all surfaces were sampled with 4×8×1 Monkhorst-Pack *k*-points.[3] The kinetic energy cutoff for plane-wave basis sets was 500 eV. The atomic cores were described by ultrasoft pseudopotentials.[4] The electronic occupation of Kohn-Sham eigenstates was smeared by the Fermi-Dirac approach with width of 0.2 eV to aid in SCF convergence for metallic systems, and all energies were extrapolated to $T = 0$ K. All calculation parameters were chosen to ensure that adsorption energies are converged within 0.1 eV.

## 2. Binding Energies of Surface Intermediates

Throughout this study, we followed the adsorption energy convention[5] for all adsorbed species ($*C_xH_yO_z$) as the difference between the electronic energy of the adsorbate-slab complex and the sum of the electronic energies of the reference slab and all adsorbate-contained atoms (C, H, and O):

$$\Delta E_{*C_xH_yO_z} = E_{*C_xH_yO_z/slab} - (E_{slab} + xE_C + yE_H + zE_O) \quad (S1)$$

where $E_{*CxHyOz/slab}$, $E_{slab}$, $E_C$, $E_H$, and $E_O$ are the electronic energies of adsorbate/slab complex, reference slab, C, H, and O atoms. The energies of C, H, and O atoms were calculated from the electronic energies of gas phase $H_2O$, $H_2$, and CO. The reference slab is the surface with specific *CO coverage. The electronic energy of a gas phase CO molecule was added by +0.20 eV to correct the limitation of PBE functional[6,7] (see Table S1).

## 3. Computational Hydrogen Electrode

The potential-dependence of reaction free energies in elementary steps involving proton-electron transfers was evaluated using the computational hydrogen electrode (CHE) approach.[8] In this approach, a reversible hydrogen electrode (RHE) is used as the reference:

$$\frac{1}{2}H_2(g) \leftrightarrow H^+(aq) + e^- \quad (S2)$$

where the proton-electron pairs are in equilibrium with $H_2$ at all values of pH and 1 *atm* of $H_2$, without potential bias. At a finite external potential $U$ vs RHE, the chemical potential of a proton-electron pair would be shifted by $-eU$, so we have,

$$\mu(H^+ + e^-) = \frac{1}{2}\mu(H_2) - eU \quad (S3)$$

For a given elementary step involving a proton-electron pair, for example,

$$A + (H^+ + e^-) \rightarrow AH \quad (S4)$$

the reaction free energy of this step at the external potential $U$ can be calculated as:

$$\Delta G_U = \Delta G_0 - (-eU) \quad (S5)$$

where $\Delta G_0$ is the reaction free energy at 0 V vs RHE. The theoretical limiting potential ($U_L$) for this elementary step, defined as the least external potential (vs RHE) required making the step exergonic, was calculated as:

$$U_L = \frac{-\Delta G_{U=0}}{e} \quad (S6)$$

The theoretical onset potential of a reaction pathway is then taken as the most negative limiting potential of ($U_L$) along the full path.

**4. Free Energies of Gas/Liquid Phase Molecules and Adsorbed Species**

Free energies of gas/liquid phase molecules and reaction intermediates were determined by incorporating corrections to the DFT-calculated electronic energies.

For gas/liquid phase molecules, we have,

$$G = E_{DFT} + E_{corr} + ZPE - TS + E_{liquid} \quad (S7)$$

Electronic energies correction ($E_{corr}$) was considered for CO and $CO_2$ to correct the limitation of PBE functional.[6,7] Zero-point energy (ZPE) was calculated from vibrational frequencies analysis with harmonic oscillator approximation and entropy corrections were calculated using ASE Thermochemistry package with the ideal gas approximation at 298.15 K and 1 *atm*. All values are similar to that obtained from standard thermodynamic tables.[9] Liquid-phase correction was added to liquid $H_2O$. The correction values are summarized in Table S1.

Similarly, for surface intermediates, we have,

$$G = E_{DFT} + ZPE - TS + E_{sol} \quad (S8)$$

The zero-point energy (ZPE) and entropy corrections, if not available from literature, were then obtained from vibrational frequencies analysis with harmonic oscillator approximation using ASE Thermochemistry package.[10] Solvation corrections were taken from the previous report.[7] The correction values for adsorbed species are summarized in Table S2.

5. **Determining CO Equilibrium Line on Reactivity Volcano**

The CO desorption line is positioned at which *CO is in equilibrium with gas phase CO (0.01 *atm*, 298.15 K), i.e., the reaction free energy $\Delta G$ is zero for the following reaction:

$$CO(g, 0.01\ atm) + * \leftrightarrow {}^{*}CO \quad (S9)$$

The corresponding binding energy of *CO can then be calculated by solving the following equation:

$$\Delta G = \Delta G^o - k_B T ln\left(\frac{P}{P^o}\right) = 0 \quad (S10)$$

where $\Delta G^o$ can be calculated as,

$$\Delta G^o = \Delta E_{*CO} + \Delta ZPE - T\Delta S^o \quad (S11)$$

From Table S1 and S2, the free energy corrections ($\Delta ZPE - T\Delta S^o$) is 0.38 eV. The surface *CO coverage estimated from the Langmuir isotherm is very low toward the right leg of the activity volcano at 0.01 atm CO. To adjust adsorbate-adsorbate interaction at 1/8 ML coverage, an extra correction to *CO binding energy was added with -0.07 eV which is the difference of *CO

binding energy at 1/8 ML coverage (-0.63 eV, calculated in this work) from experimental measurement at 0 ML limit (-0.70 eV[11]). Then, we have,

$$\Delta E_{*CO,\ 1/8ML} + (-0.07) + 0.38 - 8.62\times10^{-5}\times298.15\times ln\left(\frac{0.01}{1.0}\right) = 0 \qquad (S12)$$

By solving Eq. *S*12, we get *CO binding energy corresponding to the desorption line as $\Delta E_{*CO,1/8ML}$ = -0.43 eV. That is, for metal surfaces with *CO binding energy weaker than -0.43 eV, gas phase CO is thermodynamically more stable than *CO.

## 6. The *d*-band Model of Chemisorption

In the *d*-band model, the interaction between an adsorbate and a metal surface is separated into two steps.[12–14] Adsorbate states first interact with delocalized *sp*-electrons which leads to the formation of adsorbate resonance states. In the subsequent step, these resonance states further interact with the *d*-states centered at the average energy of the *d*-band of the surface atoms, forming bonding and anti-bonding orbitals. So the total adsorption energy can be written as,

$$\Delta E = \Delta E_{sp} + \Delta E_d \qquad (S13)$$

The interaction energy of adsorbate valence orbitals with the free-electron-like *sp*-states (the first term in Eq. *S*13) can be assumed to be approximatelly constant for different transition metals and alloys. This implies that the main difference is from the interaction of adsorbate resonance states with the *d*-band of the substrates (the second term in Eq. *S*13).

For CO chemisorption on metal surfaces, the occupied 5σ and unoccupied $2\pi^*$ orbitals participate in this process. The interactions of the resonance 5σ and $2\pi^*$ orbitals with the *d*-band of metal surfaces can be described, using the tight-binding approximation, as,

$$\Delta E_d \approx -4\left[ f\frac{V_{2\pi^*}^2}{|\varepsilon_{2\pi^*} - \varepsilon_d|} + fS_{2\pi^*}V_{2\pi^*} \right] - 2\left[ (1-f)\frac{V_{5\sigma}^2}{|\varepsilon_{5\sigma} - \varepsilon_d|} + (1+f)S_{5\sigma}V_{5\sigma} \right]. \qquad (S14)$$

The first term in each bracket describes the covalent attraction between metal *d*-states and the adsorbate orbitals, while the second term describes the Pauli repulsion when two electron clouds are brought together. The coefficient in front of the bracket is the degeneracy of the corresponding adsorbate orbitals. *f* and $\varepsilon_d$ are the filling and center of the *d*-band projected onto the surface metal atoms, respectively. $\varepsilon_{5\sigma}$ and $\varepsilon_{2\pi^*}$ are the energy levels of the renormalized adsorbate resonance orbitals formed after the interaction with the broad, free-electron-like substrate *sp*-band. To obtain those energy levels, we performed DFT calculations analyzing the adsorption of the CO on Al(100). We chose Al since it has no valance *d* electrons and its density of states distribution is broad and featureless, similar to that of the *sp* band of transition metals. We found that the occupied 5σ centers at around -7.25 eV below the Fermi level, while the unoccupied $2\pi^*$ state is around 1.32 eV above the Fermi level. *S* and *V* are the overlap integral and coupling matrix element describing the interaction between renormalized adsorbate orbitals and metal *d*-orbitals, respectively. $V_{5\sigma}$ can be approximated as $1.3V_{2\pi^*}$ based on symmetry of orbitals.[14] Furthermore, we assume that the coupling matrix element *V* is linearly related to the overlap integral *S*, i.e., $S$=-$\alpha V$, where α is an adsorbate-dependent parameter related to the repulsive interaction between coupling orbitals. We will treat α as a fitting parameter.

To obtain the absolute value of *V*, the interatomic coupling matrix element that captures the hybridization between the metal *d*-orbitals and the adsorbate orbitals, we used the relationship, $V_{2\pi*}^2 = \beta V_{ad}^2$. Here $V_{ad}^2$ is the relative coupling matrix element which is a propery of the metal.

$V_{ad}$ can be calculated in an LMTO (linear muffin tin orbital) framework. We used $V_{ad}$ tabulated in the Solid state tables.[15] $V_{ad}$ describes the relative hybridization of an adsorbate with the metal states at a fixed metal-adsorbate bond distance, while the paramter β accounts for the fact that on different metals the bonding geometry (distance, angle, etc) is different. We define β as,

$$\beta = \beta_0 \cdot \left( \frac{d_0}{d_{Cu}} \right)^7 \qquad (S15)$$

where $\beta_0$ is an adsorbate-dependent, metal-independent parameter and $d_{Cu}$ is the adsorbate bond distance to pure Cu surface in normal direction and $d_0$ is the adsorbate bond distance to bonding metal *M* regardless of metals or alloys. In the calculations below, we treat $\beta_0$ as another fitting paramter and use DFT-calculated $d_{Cu}$ and $d_0$. The $\alpha$=0.105 $eV^{-1}$, $\beta_0$=0.86 $eV^2$, and $\Delta E_{sp}$=-0.91 eV in the model is estimated by fitting the Eq. 13-15 with DFT-calculated adsorption energies of CO on designated metal and alloy surfaces. Those parameters are similar to those obtained previously[14] for CO adsorption on the {111} facet of metals and all of which are of the right order of magnitude compared to DFT estimates of 0.09 $eV^{-1}$, 2 $eV^2$, and -1.2 eV (CO adsorption energy on Al(100) surface).

**Table S1** Electronic and free energy corrections for non-adsorbed species. All corrections were determined at 298.15 K. The electronic energies correction ($E_{corr}$) of CO and $CO_2$ were calculated in the same manner as in the previous report[7] in order to adjust the limitation of PBE functional.[6]

| Species | *E*corr (eV) | ZPE (eV) | -*T*S (eV) | Liquid-phase correction (eV) |
|---|---|---|---|---|
| $CO_{(g)}$ | 0.20 | 0.15 | -0.61 | / |
| $H_{2(g)}$ | / | 0.27 | -0.40 | / |
| $H_2O_{(g)}$ | / | 0.56 | -0.58 | / |
| $CO_{2(g)}$ | 0.25 | 0.31 | -0.66 | / |
| $H_2O_{(l)}$ | / | 0.56 | -0.58 | -0.09 |

**Table S2** Free energy corrections for adsorbed species. All corrections were determined at 298.15 K. ZPE and *T*S correction values for *COOH and *CHO were calculated in this study, and other values were taken from literature.[7]

| Species | ZPE (eV) | -TS (eV) | Solvation (eV) |
|---|---|---|---|
| *COOH | 0.48 | -0.07 | -0.38 |
| *CO | 0.18 | -0.16 | -0.10 |
| *COCOH | 0.70 | -0.24 | -0.48 |
| *CHO | 0.35 | -0.06 | -0.10 |

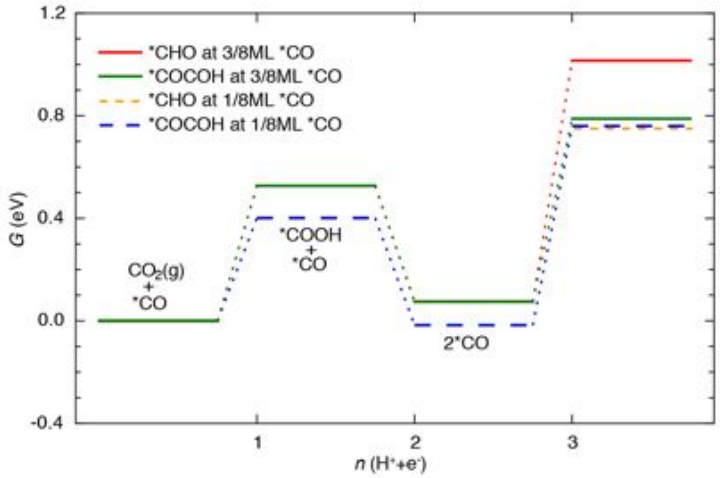



**Figure S1.** Free energy diagrams of $CO_2$ electroreduction pathways on Cu(100) with 1/8 ML and 3/8 ML initial *CO coverage.

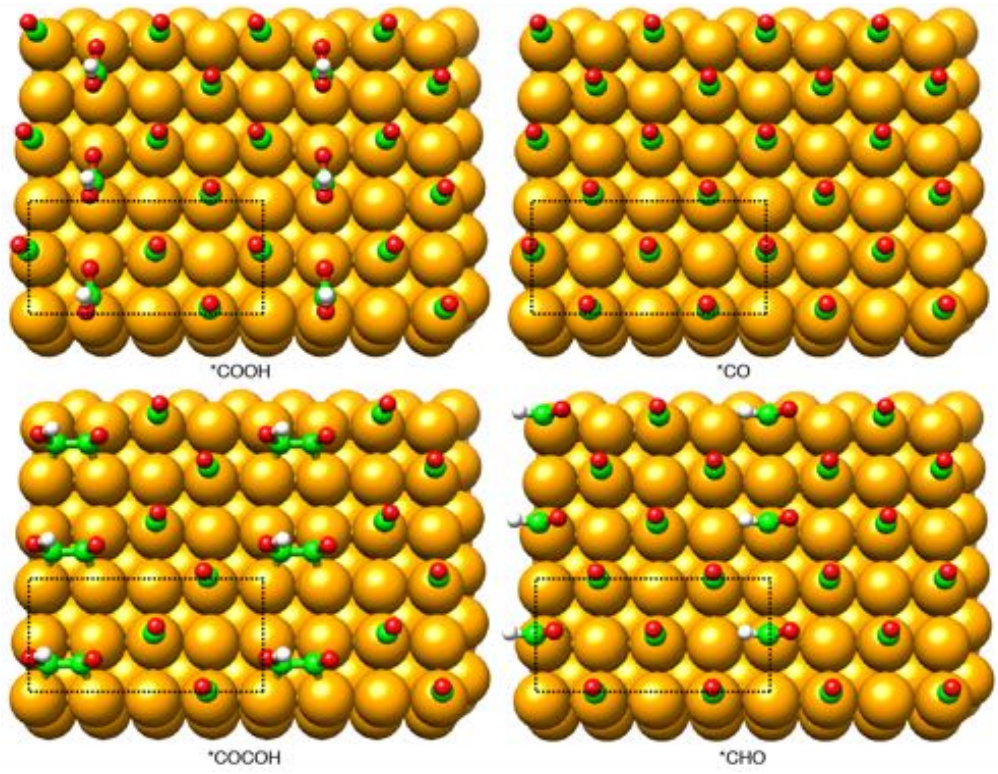



**Figure S2.** Geometric structures of adsorbed intermediates with co-adsorbed *CO on Cu(100). The unit cell is shown in black lines.

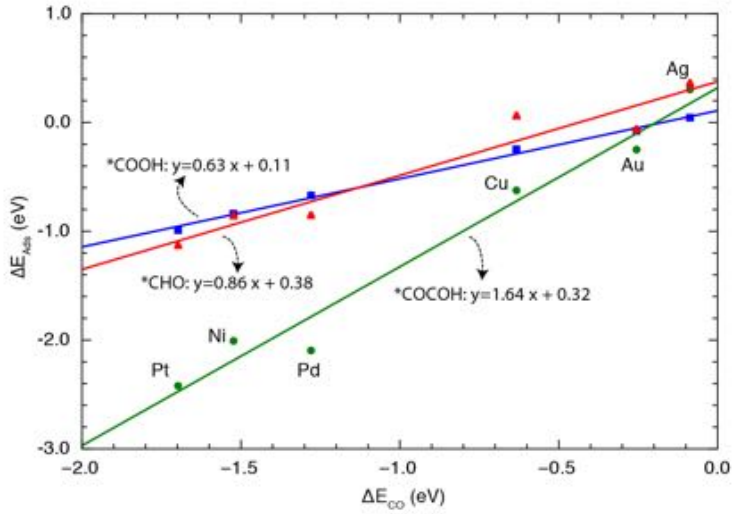
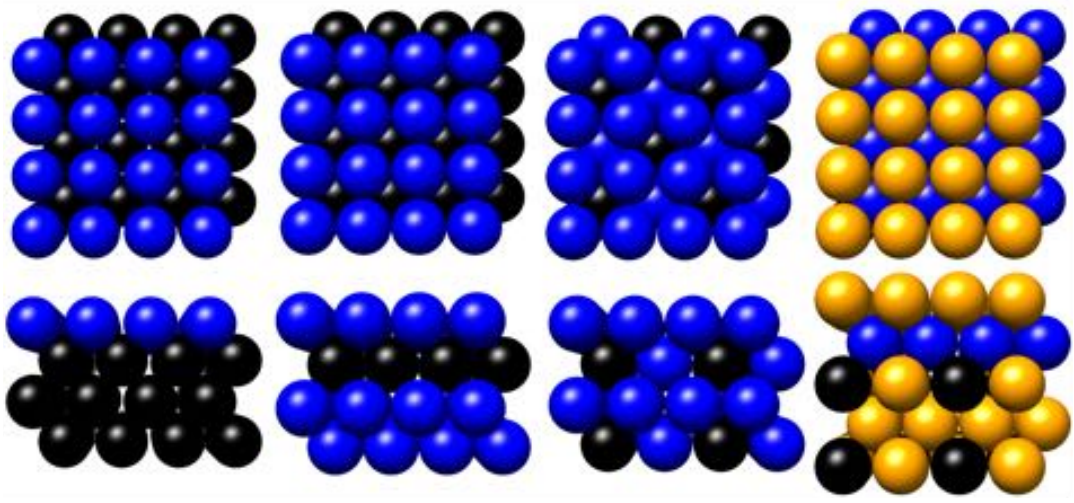



**Figure S3.** Scaling correlations of binding energies between adsorbed intermediates and *CO. The scaling equations were obtained by the linear regression method.



(a) (b) (c) (d)

**Figure S4.** Structures of {100}-terminated alloy models used in this study. (a) B@A, (b) A-B@A, (c) $A_3B$@A, and (d) $Cu_3B$-A@$Cu_{ML}$. The first and second rows are top and side views of the structures, respectively. Group VIII and IB metals (Cu, Ag, Au, Ni, Pd, and Pt) were selected for both element A and B in the B@A structure. In all other model structures, the *d*-block and post transition metals were considered for B, and A contains the group VIII and IB metals.

**Table S3**. Input features and CO adsorption energies on bimetallic surfaces for machine learning

$\Delta E_{*CO}$ : Binding energy of adsorbed CO on a metal surface

$f$ : Filling of a *d*-band

$\varepsilon_d$ : Center of a *d*-band

$W_d$ : Width of a *d*-band

$\gamma_1$ : Skewness of a *d*-band

$\gamma_2$ : Kurtosis of a *d*-band

$W$ : Work function

$r_0$ : Atomic radius

$r_d$ : Spatial extent of *d*-orbitals

IE : Ionization potential

EA : Electron affinity

$\chi_0$ : Pauling electronegativity

$\chi$ : Local Pauling electronegativity

$V_{ad}^2$ : Adsorbate-metal interatomic *d* coupling matrix element squared[15]

| Alloy Symbol | $\Delta E_{*CO}$ (eV) | $f$ | $\varepsilon_d$ (eV) | $W_d$ (eV) | $\gamma_1$ | $\gamma_2$ | $W$ (eV) | $r_0$ (Å) | $r_d$ (Å) | IE (eV) | $EA$ (eV) | $\chi_0$ | $\chi$ | $V_{ad}^2$ |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Ni@Cu | -0.69 | 0.97 | -2.21 | 1.11 | 1.08 | 8.87 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.90 | 1.00 |
| Cu@Cu | -0.63 | 0.97 | -2.25 | 1.05 | 1.13 | 10.94 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.90 | 1.00 |
| Pd@Cu | -0.86 | 0.98 | -1.66 | 0.97 | 0.47 | 8.60 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 2.03 | 1.00 |
| Ag@Cu | -0.74 | 0.98 | -1.90 | 0.88 | 0.06 | 15.15 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.91 | 1.00 |
| Ir@Cu | -0.91 | 0.97 | -2.10 | 1.13 | 0.26 | 8.42 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 2.03 | 1.00 |
| Pt@Cu | -0.91 | 0.97 | -1.85 | 1.09 | 0.03 | 8.18 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 2.06 | 1.00 |
| Au@Cu | -0.86 | 0.98 | -1.98 | 1.02 | -0.42 | 10.94 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 2.16 | 1.00 |
| Pd@Ag | -0.14 | 0.98 | -3.64 | 1.22 | 1.97 | 11.27 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 2.05 | 2.26 |
| Ag@Ag | -0.09 | 0.98 | -3.92 | 1.10 | 2.38 | 16.87 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 1.93 | 2.26 |
| Ir@Ag | -0.25 | 0.98 | -3.81 | 1.36 | 1.65 | 9.62 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 2.05 | 2.26 |
| Pt@Ag | -0.24 | 0.98 | -3.69 | 1.28 | 1.75 | 10.39 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 2.08 | 2.26 |
| Au@Ag | -0.15 | 0.98 | -3.87 | 1.16 | 1.93 | 13.38 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 2.18 | 2.26 |
| Cu@Au | -0.66 | 0.96 | -3.88 | 1.90 | 0.85 | 5.14 | 6.01 | 1.59 | 1.01 | 9.23 | 2.31 | 2.54 | 2.23 | 3.35 |
| Pd@Au | -0.27 | 0.97 | -3.07 | 1.52 | 1.02 | 5.86 | 6.01 | 1.59 | 1.01 | 9.23 | 2.31 | 2.54 | 2.38 | 3.35 |
| Ag@Au | -0.15 | 0.97 | -3.21 | 1.34 | 1.22 | 8.47 | 6.01 | 1.59 | 1.01 | 9.23 | 2.31 | 2.54 | 2.25 | 3.35 |
| Ir@Au | -0.37 | 0.96 | -3.41 | 1.72 | 0.89 | 5.32 | 6.01 | 1.59 | 1.01 | 9.23 | 2.31 | 2.54 | 2.38 | 3.35 |
| Pt@Au | -0.40 | 0.97 | -3.17 | 1.59 | 0.91 | 5.62 | 6.01 | 1.59 | 1.01 | 9.23 | 2.31 | 2.54 | 2.42 | 3.35 |
| Au@Au | -0.26 | 0.97 | -3.18 | 1.41 | 0.92 | 7.01 | 6.01 | 1.59 | 1.01 | 9.23 | 2.31 | 2.54 | 2.54 | 3.35 |
| Ni@Ni | -1.52 | 0.87 | -1.32 | 1.33 | 0.36 | 5.23 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.91 | 1.16 |
| Cu@Ni | -1.60 | 0.88 | -1.01 | 1.22 | 0.39 | 7.10 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.91 | 1.16 |
| Pd@Ni | -1.64 | 0.87 | -1.13 | 1.22 | 0.06 | 5.79 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 2.03 | 1.16 |
| Ag@Ni | -1.73 | 0.88 | -0.77 | 1.05 | -0.37 | 11.06 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.92 | 1.16 |
| Ir@Ni | -1.59 | 0.87 | -1.21 | 1.36 | -0.31 | 6.48 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 2.03 | 1.16 |

| | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Pt@Ni | -1.63 | 0.88 | -1.24 | 1.34 | -0.28 | 6.05 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 2.07 | 1.16 |
| Au@Ni | -1.80 | 0.88 | -0.87 | 1.19 | -0.80 | 9.02 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 2.17 | 1.16 |
| Cu@Pd | -0.84 | 0.93 | -2.05 | 1.62 | 0.25 | 3.27 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.06 | 2.78 |
| Pd@Pd | -1.28 | 0.92 | -1.67 | 1.36 | 0.23 | 3.93 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.20 | 2.78 |
| Ag@Pd | -1.12 | 0.93 | -1.31 | 1.23 | 0.02 | 6.87 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.08 | 2.78 |
| Ir@Pd | -1.18 | 0.91 | -2.15 | 1.60 | 0.14 | 3.98 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.20 | 2.78 |
| Pt@Pd | -1.31 | 0.92 | -1.82 | 1.48 | 0.05 | 4.32 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.24 | 2.78 |
| Au@Pd | -1.29 | 0.93 | -1.35 | 1.35 | -0.21 | 5.94 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.35 | 2.78 |
| Cu@Pt | -1.11 | 0.89 | -2.33 | 2.05 | 0.14 | 2.75 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.10 | 3.90 |
| Pd@Pt | -1.66 | 0.88 | -1.90 | 1.74 | 0.27 | 3.46 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.24 | 3.90 |
| Ag@Pt | -1.59 | 0.90 | -1.38 | 1.52 | 0.14 | 5.03 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.12 | 3.90 |
| Ir@Pt | -1.49 | 0.88 | -2.37 | 2.04 | 0.21 | 3.35 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.24 | 3.90 |
| Pt@Pt | -1.70 | 0.88 | -2.03 | 1.87 | 0.17 | 3.65 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.28 | 3.90 |
| Au@Pt | -1.84 | 0.90 | -1.46 | 1.64 | -0.06 | 4.52 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.39 | 3.90 |
| Cu-Sc@Cu | -0.63 | 0.97 | -2.72 | 0.99 | 2.79 | 16.86 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.64 | 1.00 |
| Cu-Ti@Cu | -0.69 | 0.97 | -2.83 | 1.02 | 2.48 | 14.50 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.73 | 1.00 |
| Cu-V@Cu | -0.81 | 0.97 | -2.74 | 1.07 | 2.12 | 11.81 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.77 | 1.00 |
| Cu-Cr@Cu | -1.17 | 0.97 | -2.59 | 1.10 | 1.71 | 9.68 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.79 | 1.00 |
| Cu-Co@Cu | -0.76 | 0.97 | -2.34 | 1.08 | 1.28 | 9.60 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.89 | 1.00 |
| Cu-Ni@Cu | -0.72 | 0.97 | -2.14 | 1.07 | 1.25 | 9.36 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.90 | 1.00 |
| Cu-Cu@Cu | -0.63 | 0.97 | -2.26 | 1.06 | 1.11 | 10.84 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.90 | 1.00 |
| Cu-Y@Cu | -0.73 | 0.97 | -2.56 | 0.96 | 2.76 | 17.57 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.56 | 1.00 |
| Cu-Zr@Cu | -0.84 | 0.97 | -2.74 | 1.02 | 2.58 | 15.81 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.62 | 1.00 |
| Cu-Nb@Cu | -1.05 | 0.97 | -2.71 | 1.08 | 2.14 | 12.69 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.76 | 1.00 |
| Cu-Mo@Cu | -1.18 | 0.97 | -2.52 | 1.11 | 1.58 | 9.93 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 2.01 | 1.00 |
| Cu-Ru@Cu | -0.87 | 0.97 | -2.31 | 1.08 | 0.94 | 8.48 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 2.03 | 1.00 |
| Cu-Rh@Cu | -0.81 | 0.97 | -2.14 | 1.07 | 0.85 | 8.58 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 2.06 | 1.00 |
| Cu-Pd@Cu | -0.75 | 0.97 | -1.99 | 1.03 | 0.71 | 9.38 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 2.03 | 1.00 |
| Cu-Ag@Cu | -0.64 | 0.98 | -2.13 | 0.98 | 0.68 | 14.09 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.91 | 1.00 |
| Cu-La@Cu | -0.69 | 0.97 | -2.41 | 0.93 | 2.54 | 19.64 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.49 | 1.00 |
| Cu-Ta@Cu | -1.01 | 0.97 | -2.83 | 1.14 | 2.06 | 12.45 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.71 | 1.00 |
| Cu-W@Cu | -1.18 | 0.97 | -2.63 | 1.19 | 1.46 | 9.55 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 2.09 | 1.00 |
| Cu-Re@Cu | -1.12 | 0.97 | -2.64 | 1.21 | 0.96 | 8.28 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.90 | 1.00 |
| Cu-Os@Cu | -0.90 | 0.97 | -2.52 | 1.19 | 0.68 | 7.98 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 2.03 | 1.00 |
| Cu-Ir@Cu | -0.78 | 0.97 | -2.31 | 1.16 | 0.47 | 8.28 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 2.03 | 1.00 |
| Cu-Pt@Cu | -0.79 | 0.97 | -2.09 | 1.12 | 0.28 | 8.95 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 2.06 | 1.00 |
| Cu-Au@Cu | -0.67 | 0.98 | -2.08 | 1.04 | 0.13 | 12.70 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 2.16 | 1.00 |
| Ag-Sc@Ag | -0.06 | 0.98 | -4.49 | 1.17 | 3.84 | 22.63 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 1.65 | 2.26 |
| Ag-Ti@Ag | -0.15 | 0.98 | -4.41 | 1.16 | 3.51 | 20.02 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 1.75 | 2.26 |
| Ag-Ni@Ag | -0.14 | 0.98 | -3.73 | 1.20 | 2.66 | 14.40 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 1.92 | 2.26 |
| Ag-Cu@Ag | -0.06 | 0.98 | -4.01 | 1.18 | 2.61 | 15.30 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 1.92 | 2.26 |
| Ag-Y@Ag | -0.11 | 0.98 | -4.36 | 1.14 | 4.02 | 24.83 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 1.57 | 2.26 |
| Ag-Zr@Ag | -0.13 | 0.97 | -4.42 | 1.21 | 3.68 | 20.94 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 1.64 | 2.26 |
| Ag-Nb@Ag | -0.24 | 0.97 | -4.33 | 1.26 | 3.24 | 16.96 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 1.78 | 2.26 |
| Ag-Pd@Ag | -0.15 | 0.98 | -3.50 | 1.13 | 2.35 | 13.34 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 2.05 | 2.26 |
| Ag-Ag@Ag | -0.09 | 0.98 | -3.92 | 1.10 | 2.38 | 16.87 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 1.93 | 2.26 |
| Ag-La@Ag | -0.12 | 0.98 | -4.15 | 1.06 | 4.06 | 27.12 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 1.93 | 2.26 |

| | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Ag-Ta@Ag | -0.27 | 0.97 | -4.41 | 1.35 | 3.06 | 15.39 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 1.73 | 2.26 |
| Ag-Pt@Ag | -0.23 | 0.98 | -3.55 | 1.23 | 1.96 | 10.78 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 2.08 | 2.26 |
| Ag-Au@Ag | -0.12 | 0.98 | -3.86 | 1.17 | 1.88 | 13.13 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 2.18 | 2.26 |
| Au-Cu@Au | -0.11 | 0.97 | -3.40 | 1.45 | 1.41 | 7.73 | 6.01 | 1.59 | 1.01 | 9.23 | 2.31 | 2.54 | 2.23 | 3.35 |
| Au-Y@Au | -0.10 | 0.96 | -4.01 | 1.47 | 2.63 | 12.80 | 6.01 | 1.59 | 1.01 | 9.23 | 2.31 | 2.54 | 1.83 | 3.35 |
| Au-Ru@Au | -0.47 | 0.96 | -3.35 | 1.49 | 1.39 | 6.53 | 6.01 | 1.59 | 1.01 | 9.23 | 2.31 | 2.54 | 2.38 | 3.35 |
| Au-Pd@Au | -0.39 | 0.97 | -2.89 | 1.39 | 1.19 | 6.40 | 6.01 | 1.59 | 1.01 | 9.23 | 2.31 | 2.54 | 2.38 | 3.35 |
| Au-Ag@Au | -0.18 | 0.97 | -3.19 | 1.32 | 1.25 | 8.65 | 6.01 | 1.59 | 1.01 | 9.23 | 2.31 | 2.54 | 2.25 | 3.35 |
| Au-La@Au | -0.11 | 0.96 | -3.71 | 1.36 | 2.49 | 13.27 | 6.01 | 1.59 | 1.01 | 9.23 | 2.31 | 2.54 | 1.75 | 3.35 |
| Au-Pt@Au | -0.51 | 0.97 | -3.01 | 1.49 | 1.02 | 5.76 | 6.01 | 1.59 | 1.01 | 9.23 | 2.31 | 2.54 | 2.42 | 3.35 |
| Au-Au@Au | -0.26 | 0.97 | -3.18 | 1.41 | 0.92 | 7.01 | 6.01 | 1.59 | 1.01 | 9.23 | 2.31 | 2.54 | 2.54 | 3.35 |
| Ni-Sc@Ni | -1.27 | 0.88 | -1.22 | 1.28 | 1.46 | 7.33 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.64 | 1.16 |
| Ni-Ti@Ni | -1.30 | 0.88 | -1.36 | 1.33 | 1.19 | 6.16 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.74 | 1.16 |
| Ni-V@Ni | -1.36 | 0.87 | -1.43 | 1.36 | 0.90 | 5.19 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.78 | 1.16 |
| Ni-Cr@Ni | -1.39 | 0.87 | -1.53 | 1.38 | 0.67 | 4.78 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.79 | 1.16 |
| Ni-Co@Ni | -1.45 | 0.87 | -1.44 | 1.37 | 0.40 | 5.09 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.90 | 1.16 |
| Ni-Ni@Ni | -1.52 | 0.87 | -1.32 | 1.33 | 0.36 | 5.23 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.91 | 1.16 |
| Ni-Cu@Ni | -1.54 | 0.88 | -1.11 | 1.26 | 0.31 | 6.41 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.91 | 1.16 |
| Ni-Y@Ni | -1.23 | 0.88 | -1.10 | 1.20 | 1.37 | 7.88 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.56 | 1.16 |
| Ni-Zr@Ni | -1.33 | 0.88 | -1.19 | 1.27 | 1.23 | 7.16 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.63 | 1.16 |
| Ni-Nb@Ni | -1.47 | 0.87 | -1.27 | 1.37 | 1.02 | 6.38 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.77 | 1.16 |
| Ni-Mo@Ni | -1.65 | 0.87 | -1.35 | 1.40 | 0.64 | 5.57 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 2.02 | 1.16 |
| Ni-Ru@Ni | -1.87 | 0.87 | -1.35 | 1.36 | 0.03 | 5.36 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 2.03 | 1.16 |
| Ni-Rh@Ni | -1.73 | 0.87 | -1.30 | 1.34 | 0.00 | 5.40 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 2.07 | 1.16 |
| Ni-Pd@Ni | -1.68 | 0.87 | -1.22 | 1.27 | 0.03 | 5.82 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 2.03 | 1.16 |
| Ni-Ag@Ni | -1.61 | 0.88 | -1.08 | 1.18 | 0.04 | 8.36 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.92 | 1.16 |
| Ni-Ta@Ni | -1.44 | 0.88 | -1.35 | 1.43 | 0.96 | 6.34 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.72 | 1.16 |
| Ni-W@Ni | -1.62 | 0.87 | -1.43 | 1.50 | 0.63 | 5.73 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 2.10 | 1.16 |
| Ni-Re@Ni | -1.75 | 0.87 | -1.50 | 1.54 | 0.22 | 5.31 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.91 | 1.16 |
| Ni-Os@Ni | -1.87 | 0.87 | -1.50 | 1.53 | -0.13 | 5.45 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 2.03 | 1.16 |
| Ni-Ir@Ni | -1.80 | 0.87 | -1.36 | 1.45 | -0.38 | 6.06 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 2.03 | 1.16 |
| Ni-Pt@Ni | -1.74 | 0.87 | -1.28 | 1.36 | -0.33 | 6.43 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 2.07 | 1.16 |
| Ni-Au@Ni | -1.71 | 0.87 | -1.08 | 1.24 | -0.31 | 8.68 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 2.17 | 1.16 |
| Pd-Sc@Pd | -0.48 | 0.92 | -2.39 | 1.50 | 1.69 | 7.11 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 1.78 | 2.78 |
| Pd-Ti@Pd | -0.53 | 0.93 | -2.56 | 1.51 | 1.41 | 5.85 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 1.88 | 2.78 |
| Pd-V@Pd | -0.61 | 0.91 | -2.53 | 1.54 | 1.17 | 4.95 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 1.93 | 2.78 |
| Pd-Mn@Pd | -0.68 | 0.92 | -2.03 | 1.49 | 0.89 | 4.98 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 1.88 | 2.78 |
| Pd-Co@Pd | -0.90 | 0.92 | -2.06 | 1.47 | 0.58 | 4.31 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.05 | 2.78 |
| Pd-Ni@Pd | -1.05 | 0.92 | -1.90 | 1.43 | 0.55 | 4.25 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.07 | 2.78 |
| Pd-Cu@Pd | -1.12 | 0.93 | -1.64 | 1.38 | 0.38 | 4.28 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.06 | 2.78 |
| Pd-Y@Pd | -0.55 | 0.92 | -2.17 | 1.41 | 1.64 | 7.41 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 1.69 | 2.78 |
| Pd-Zr@Pd | -0.62 | 0.92 | -2.32 | 1.55 | 1.60 | 6.93 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 1.76 | 2.78 |
| Pd-Nb@Pd | -0.72 | 0.92 | -2.47 | 1.62 | 1.31 | 5.56 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 1.91 | 2.78 |
| Pd-Mo@Pd | -0.79 | 0.91 | -2.46 | 1.61 | 0.99 | 4.53 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.18 | 2.78 |
| Pd-Ru@Pd | -1.09 | 0.91 | -2.16 | 1.51 | 0.49 | 3.74 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.20 | 2.78 |
| Pd-Rh@Pd | -1.18 | 0.91 | -1.99 | 1.47 | 0.40 | 3.84 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.24 | 2.78 |
| Pd-Pd@Pd | -1.28 | 0.92 | -1.67 | 1.36 | 0.23 | 3.93 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.20 | 2.78 |

| | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| Pd-Ag@Pd | -1.16 | 0.93 | -1.40 | 1.28 | -0.02 | 5.13 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.08 | 2.78 |
| Pd-La@Pd | -0.50 | 0.92 | -1.96 | 1.32 | 1.28 | 8.09 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 1.62 | 2.78 |
| Pd-Ta@Pd | -0.74 | 0.92 | -2.59 | 1.71 | 1.33 | 5.79 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 1.86 | 2.78 |
| Pd-W@Pd | -0.80 | 0.91 | -2.67 | 1.75 | 1.02 | 4.70 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.27 | 2.78 |
| Pd-Os@Pd | -1.05 | 0.91 | -2.50 | 1.71 | 0.42 | 3.71 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.20 | 2.78 |
| Pd-Ir@Pd | -1.23 | 0.91 | -2.23 | 1.63 | 0.21 | 3.76 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.20 | 2.78 |
| Pd-Pt@Pd | -1.33 | 0.92 | -1.82 | 1.49 | 0.03 | 4.01 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.24 | 2.78 |
| Pd-Au@Pd | -1.31 | 0.93 | -1.51 | 1.39 | -0.19 | 5.01 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.35 | 2.78 |
| Pt-Sc@Pt | -0.68 | 0.89 | -2.46 | 1.90 | 1.31 | 5.16 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 1.81 | 3.90 |
| Pt-Ti@Pt | -0.77 | 0.89 | -2.70 | 1.90 | 1.11 | 4.51 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 1.92 | 3.90 |
| Pt-V@Pt | -0.88 | 0.88 | -2.65 | 1.93 | 0.90 | 3.93 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 1.96 | 3.90 |
| Pt-Co@Pt | -1.18 | 0.88 | -2.12 | 1.81 | 0.50 | 3.77 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.09 | 3.90 |
| Pt-Ni@Pt | -1.36 | 0.88 | -2.05 | 1.80 | 0.46 | 3.68 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.11 | 3.90 |
| Pt-Cu@Pt | -1.44 | 0.89 | -1.76 | 1.74 | 0.36 | 3.88 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.10 | 3.90 |
| Pt-Y@Pt | -0.79 | 0.88 | -2.33 | 1.80 | 1.31 | 5.54 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 1.73 | 3.90 |
| Pt-Zr@Pt | -0.89 | 0.88 | -2.51 | 1.95 | 1.28 | 5.14 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 1.79 | 3.90 |
| Pt-Nb@Pt | -1.06 | 0.88 | -2.60 | 2.02 | 1.04 | 4.24 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 1.95 | 3.90 |
| Pt-Mo@Pt | -1.09 | 0.88 | -2.59 | 2.01 | 0.78 | 3.64 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.23 | 3.90 |
| Pt-Ru@Pt | -1.43 | 0.87 | -2.32 | 1.88 | 0.42 | 3.34 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.24 | 3.90 |
| Pt-Rh@Pt | -1.49 | 0.88 | -2.19 | 1.84 | 0.36 | 3.45 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.28 | 3.90 |
| Pt-Pd@Pt | -1.64 | 0.88 | -1.86 | 1.71 | 0.28 | 3.65 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.24 | 3.90 |
| Pt-Ag@Pt | -1.52 | 0.90 | -1.56 | 1.62 | 0.23 | 4.47 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.12 | 3.90 |
| Pt-La@Pt | -0.72 | 0.88 | -2.05 | 1.69 | 1.01 | 5.86 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 1.65 | 3.90 |
| Pt-Ta@Pt | -1.04 | 0.88 | -2.74 | 2.15 | 1.07 | 4.36 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 1.89 | 3.90 |
| Pt-W@Pt | -1.08 | 0.87 | -2.76 | 2.16 | 0.80 | 3.71 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.32 | 3.90 |
| Pt-Re@Pt | -1.20 | 0.88 | -2.73 | 2.14 | 0.56 | 3.34 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.10 | 3.90 |
| Pt-Os@Pt | -1.40 | 0.88 | -2.65 | 2.10 | 0.37 | 3.27 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.24 | 3.90 |
| Pt-Ir@Pt | -1.52 | 0.87 | -2.41 | 2.01 | 0.25 | 3.39 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.24 | 3.90 |
| Pt-Pt@Pt | -1.70 | 0.88 | -2.03 | 1.87 | 0.17 | 3.65 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.28 | 3.90 |
| Pt-Au@Pt | -1.67 | 0.89 | -1.63 | 1.74 | 0.07 | 4.25 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.39 | 3.90 |
| $Cu_3Sc$@Cu | -0.51 | 0.97 | -2.38 | 0.91 | 2.41 | 16.40 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.76 | 1.00 |
| $Cu_3Ti$@Cu | -0.52 | 0.97 | -2.45 | 0.97 | 1.96 | 13.27 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.81 | 1.00 |
| $Cu_3V$@Cu | -0.65 | 0.97 | -2.34 | 1.00 | 1.78 | 12.24 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.84 | 1.00 |
| $Cu_3Cr$@Cu | -0.66 | 0.97 | -2.36 | 1.01 | 1.70 | 12.23 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.84 | 1.00 |
| $Cu_3Mn$@Cu | -0.63 | 0.97 | -2.38 | 1.01 | 1.55 | 12.33 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.82 | 1.00 |
| $Cu_3Co$@Cu | -0.63 | 0.97 | -2.19 | 1.07 | 1.19 | 9.91 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.90 | 1.00 |
| $Cu_3Ni$@Cu | -0.66 | 0.97 | -2.15 | 1.07 | 1.17 | 9.80 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.90 | 1.00 |
| $Cu_3Cu$@Cu | -0.63 | 0.97 | -2.26 | 1.06 | 1.11 | 10.84 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.90 | 1.00 |
| $Cu_3Zn$@Cu | -0.70 | 0.98 | -2.36 | 1.02 | 0.94 | 13.94 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.84 | 1.00 |
| $Cu_3Ga$@Cu | -0.72 | 0.97 | -2.53 | 1.06 | 0.85 | 15.36 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.88 | 1.00 |
| $Cu_3Ge$@Cu | -0.80 | 0.97 | -2.46 | 1.09 | 0.54 | 14.48 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.92 | 1.00 |
| $Cu_3Y$@Cu | -0.49 | 0.97 | -2.31 | 0.90 | 2.20 | 15.96 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.72 | 1.00 |
| $Cu_3Zr$@Cu | -0.56 | 0.97 | -2.39 | 0.93 | 2.37 | 15.68 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.76 | 1.00 |
| $Cu_3Nb$@Cu | -0.51 | 0.97 | -2.36 | 0.99 | 1.91 | 12.49 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.83 | 1.00 |
| $Cu_3Mo$@Cu | -0.48 | 0.97 | -2.27 | 1.03 | 1.51 | 10.49 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.95 | 1.00 |
| $Cu_3Ru$@Cu | -0.67 | 0.97 | -2.04 | 1.04 | 1.06 | 9.17 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.96 | 1.00 |
| $Cu_3Rh$@Cu | -0.72 | 0.97 | -1.98 | 1.04 | 0.99 | 9.29 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.98 | 1.00 |

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|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $Cu_3Pd$@Cu | -0.70 | 0.97 | -1.94 | 1.01 | 0.87 | 9.99 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.96 | 1.00 |
| $Cu_3Ag$@Cu | -0.70 | 0.98 | -2.09 | 0.96 | 0.77 | 13.51 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.91 | 1.00 |
| $Cu_3In$@Cu | -0.75 | 0.98 | -2.39 | 0.99 | -0.21 | 29.99 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.87 | 1.00 |
| $Cu_3La$@Cu | -0.60 | 0.97 | -2.16 | 0.86 | 2.11 | 16.29 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.68 | 1.00 |
| $Cu_3Ta$@Cu | -0.49 | 0.97 | -2.47 | 1.03 | 1.90 | 12.33 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.80 | 1.00 |
| $Cu_3W$@Cu | -0.46 | 0.97 | -2.38 | 1.08 | 1.49 | 10.17 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.99 | 1.00 |
| $Cu_3Re$@Cu | -0.49 | 0.97 | -2.31 | 1.13 | 1.11 | 8.69 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.90 | 1.00 |
| $Cu_3Os$@Cu | -0.65 | 0.97 | -2.23 | 1.13 | 0.92 | 8.43 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.96 | 1.00 |
| $Cu_3Ir$@Cu | -0.72 | 0.97 | -2.09 | 1.10 | 0.78 | 8.59 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.96 | 1.00 |
| $Cu_3Pt$@Cu | -0.74 | 0.97 | -1.97 | 1.07 | 0.61 | 9.16 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.98 | 1.00 |
| $Cu_3Au$@Cu | -0.72 | 0.98 | -2.11 | 1.02 | 0.35 | 11.84 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 2.03 | 1.00 |
| $Cu_3Tl$@Cu | -0.73 | 0.98 | -2.31 | 0.98 | -0.51 | 27.36 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.83 | 1.00 |
| $Cu_3Pb$@Cu | -0.80 | 0.98 | -2.27 | 0.92 | 0.77 | 19.57 | 5.30 | 1.41 | 0.67 | 7.73 | 1.24 | 1.90 | 1.99 | 1.00 |
| $Ag_3Sc$@Ag | -0.05 | 0.98 | -4.02 | 1.06 | 3.28 | 20.88 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 1.79 | 2.26 |
| $Ag_3Ti$@Ag | -0.10 | 0.98 | -4.01 | 1.09 | 2.96 | 18.67 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 1.84 | 2.26 |
| $Ag_3V$@Ag | -0.12 | 0.98 | -3.98 | 1.13 | 2.88 | 17.91 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 1.86 | 2.26 |
| $Ag_3Cr$@Ag | -0.12 | 0.98 | -4.03 | 1.13 | 2.88 | 18.26 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 1.87 | 2.26 |
| $Ag_3Mn$@Ag | -0.12 | 0.98 | -4.08 | 1.15 | 2.71 | 17.36 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 1.84 | 2.26 |
| $Ag_3Co$@Ag | -0.11 | 0.98 | -3.90 | 1.19 | 2.32 | 14.44 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 1.92 | 2.26 |
| $Ag_3Ni$@Ag | -0.09 | 0.98 | -3.85 | 1.20 | 2.29 | 14.31 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 1.93 | 2.26 |
| $Ag_3Cu$@Ag | -0.08 | 0.98 | -3.99 | 1.16 | 2.37 | 15.46 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 1.92 | 2.26 |
| $Ag_3Zn$@Ag | -0.11 | 0.98 | -4.10 | 1.14 | 2.28 | 16.76 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 1.86 | 2.26 |
| $Ag_3Ga$@Ag | -0.14 | 0.98 | -4.12 | 1.16 | 2.34 | 17.28 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 1.90 | 2.26 |
| $Ag_3Ge$@Ag | -0.20 | 0.98 | -3.92 | 1.13 | 2.25 | 17.64 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 1.95 | 2.26 |
| $Ag_3Nb$@Ag | -0.07 | 0.98 | -3.89 | 1.14 | 2.86 | 16.72 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 1.85 | 2.26 |
| $Ag_3Ru$@Ag | -0.11 | 0.98 | -3.65 | 1.18 | 2.24 | 13.22 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 1.99 | 2.26 |
| $Ag_3Pd$@Ag | -0.08 | 0.98 | -3.69 | 1.13 | 2.30 | 14.48 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 1.99 | 2.26 |
| $Ag_3Ag$@Ag | -0.09 | 0.98 | -3.92 | 1.10 | 2.38 | 16.87 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 1.93 | 2.26 |
| $Ag_3Ta$@Ag | -0.02 | 0.97 | -3.98 | 1.21 | 2.73 | 15.39 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 1.82 | 2.26 |
| $Ag_3W$@Ag | -0.03 | 0.97 | -3.89 | 1.24 | 2.47 | 13.65 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 2.02 | 2.26 |
| $Ag_3Os$@Ag | -0.10 | 0.98 | -3.74 | 1.24 | 2.10 | 11.95 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 1.99 | 2.26 |
| $Ag_3Ir$@Ag | -0.14 | 0.98 | -3.66 | 1.22 | 2.09 | 12.20 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 1.99 | 2.26 |
| $Ag_3Pt$@Ag | -0.12 | 0.98 | -3.68 | 1.18 | 2.11 | 12.89 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 2.00 | 2.26 |
| $Ag_3Au$@Ag | -0.11 | 0.98 | -3.86 | 1.13 | 2.14 | 14.93 | 5.01 | 1.59 | 0.89 | 7.58 | 1.30 | 1.93 | 2.05 | 2.26 |
| $Au_3Cu$@Au | -0.17 | 0.97 | -3.34 | 1.48 | 1.09 | 6.97 | 6.01 | 1.59 | 1.01 | 9.23 | 2.31 | 2.54 | 2.38 | 3.35 |
| $Au_3Zn$@Au | -0.24 | 0.97 | -3.50 | 1.45 | 1.00 | 7.66 | 6.01 | 1.59 | 1.01 | 9.23 | 2.31 | 2.54 | 2.31 | 3.35 |
| $Au_3Ga$@Au | -0.21 | 0.97 | -3.53 | 1.47 | 1.12 | 8.26 | 6.01 | 1.59 | 1.01 | 9.23 | 2.31 | 2.54 | 2.36 | 3.35 |
| $Au_3Pd$@Au | -0.30 | 0.97 | -2.99 | 1.43 | 1.02 | 6.49 | 6.01 | 1.59 | 1.01 | 9.23 | 2.31 | 2.54 | 2.46 | 3.35 |
| $Au_3Ag$@Au | -0.21 | 0.97 | -3.17 | 1.37 | 1.07 | 7.67 | 6.01 | 1.59 | 1.01 | 9.23 | 2.31 | 2.54 | 2.39 | 3.35 |
| $Au_3Pt$@Au | -0.36 | 0.97 | -3.02 | 1.47 | 0.94 | 6.07 | 6.01 | 1.59 | 1.01 | 9.23 | 2.31 | 2.54 | 2.48 | 3.35 |
| $Au_3Au$@Au | -0.26 | 0.97 | -3.18 | 1.41 | 0.92 | 7.01 | 6.01 | 1.59 | 1.01 | 9.23 | 2.31 | 2.54 | 2.54 | 3.35 |
| $Ni_3Sc$@Ni | -1.47 | 0.88 | -0.94 | 1.18 | 1.08 | 6.70 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.77 | 1.16 |
| $Ni_3Ti$@Ni | -1.52 | 0.88 | -1.20 | 1.30 | 0.73 | 5.38 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.82 | 1.16 |
| $Ni_3V$@Ni | -1.40 | 0.87 | -1.52 | 1.37 | 0.59 | 5.02 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.84 | 1.16 |
| $Ni_3Cr$@Ni | -1.53 | 0.87 | -1.31 | 1.33 | 0.46 | 5.11 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.85 | 1.16 |
| $Ni_3Co$@Ni | -1.47 | 0.87 | -1.42 | 1.36 | 0.37 | 5.13 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.90 | 1.16 |
| $Ni_3Ni$@Ni | -1.52 | 0.87 | -1.32 | 1.33 | 0.36 | 5.23 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.91 | 1.16 |

| | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $Ni_3Cu$@Ni | -1.52 | 0.87 | -1.19 | 1.29 | 0.34 | 5.79 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.91 | 1.16 |
| $Ni_3Zn$@Ni | -1.53 | 0.88 | -1.15 | 1.27 | 0.28 | 7.68 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.85 | 1.16 |
| $Ni_3Ga$@Ni | -1.56 | 0.88 | -1.11 | 1.32 | 0.06 | 9.93 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.89 | 1.16 |
| $Ni_3Ge$@Ni | -1.54 | 0.88 | -1.19 | 1.38 | -0.20 | 8.89 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.93 | 1.16 |
| $Ni_3Y$@Ni | -1.49 | 0.88 | -0.79 | 1.10 | 1.34 | 8.08 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.73 | 1.16 |
| $Ni_3Zr$@Ni | -1.54 | 0.88 | -1.04 | 1.23 | 0.92 | 6.07 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.76 | 1.16 |
| $Ni_3Nb$@Ni | -1.35 | 0.87 | -1.49 | 1.34 | 0.74 | 5.63 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.84 | 1.16 |
| $Ni_3Mo$@Ni | -1.36 | 0.87 | -1.52 | 1.37 | 0.51 | 5.25 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.96 | 1.16 |
| $Ni_3Ru$@Ni | -1.52 | 0.87 | -1.33 | 1.32 | 0.27 | 5.35 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.97 | 1.16 |
| $Ni_3Rh$@Ni | -1.56 | 0.87 | -1.30 | 1.32 | 0.26 | 5.41 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.99 | 1.16 |
| $Ni_3Pd$@Ni | -1.61 | 0.87 | -1.20 | 1.27 | 0.22 | 6.09 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.97 | 1.16 |
| $Ni_3Ag$@Ni | -1.62 | 0.88 | -1.10 | 1.22 | 0.18 | 7.75 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.91 | 1.16 |
| $Ni_3In$@Ni | -1.63 | 0.89 | -0.99 | 1.22 | -0.48 | 18.37 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.88 | 1.16 |
| $Ni_3Sn$@Ni | -1.63 | 0.89 | -0.98 | 1.22 | 0.11 | 9.69 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.92 | 1.16 |
| $Ni_3La$@Ni | -1.47 | 0.89 | -0.75 | 1.07 | 1.32 | 8.28 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.69 | 1.16 |
| $Ni_3Ta$@Ni | -1.33 | 0.87 | -1.54 | 1.40 | 0.76 | 5.63 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.81 | 1.16 |
| $Ni_3W$@Ni | -1.34 | 0.87 | -1.60 | 1.43 | 0.52 | 5.20 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 2.00 | 1.16 |
| $Ni_3Re$@Ni | -1.34 | 0.87 | -1.59 | 1.46 | 0.26 | 4.87 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.91 | 1.16 |
| $Ni_3Os$@Ni | -1.44 | 0.87 | -1.45 | 1.43 | 0.07 | 5.10 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.97 | 1.16 |
| $Ni_3Ir$@Ni | -1.58 | 0.87 | -1.30 | 1.37 | 0.03 | 5.60 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.97 | 1.16 |
| $Ni_3Pt$@Ni | -1.65 | 0.87 | -1.25 | 1.33 | 0.05 | 6.16 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.99 | 1.16 |
| $Ni_3Au$@Ni | -1.68 | 0.87 | -1.12 | 1.27 | -0.06 | 7.75 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 2.03 | 1.16 |
| $Ni_3Tl$@Ni | -1.68 | 0.89 | -0.97 | 1.21 | -0.69 | 17.49 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.84 | 1.16 |
| $Ni_3Pb$@Ni | -1.65 | 0.89 | -0.91 | 1.15 | -0.07 | 12.21 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 2.00 | 1.16 |
| $Ni_3Bi$@Ni | -1.63 | 0.89 | -1.04 | 1.23 | -0.57 | 15.32 | 5.77 | 1.38 | 0.71 | 7.64 | 1.16 | 1.91 | 1.93 | 1.16 |
| $Pd_3Sc$@Pd | -0.82 | 0.93 | -1.72 | 1.39 | 1.04 | 5.49 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 1.98 | 2.78 |
| $Pd_3Ti$@Pd | -0.94 | 0.93 | -2.27 | 1.51 | 0.78 | 4.33 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.03 | 2.78 |
| $Pd_3V$@Pd | -0.95 | 0.92 | -2.19 | 1.51 | 0.64 | 4.06 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.06 | 2.78 |
| $Pd_3Cr$@Pd | -0.99 | 0.92 | -1.87 | 1.43 | 0.58 | 4.23 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.07 | 2.78 |
| $Pd_3Mn$@Pd | -1.00 | 0.93 | -1.75 | 1.41 | 0.53 | 4.39 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.04 | 2.78 |
| $Pd_3Co$@Pd | -1.07 | 0.92 | -1.95 | 1.48 | 0.35 | 3.80 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.12 | 2.78 |
| $Pd_3Ni$@Pd | -1.17 | 0.92 | -1.82 | 1.43 | 0.35 | 3.86 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.13 | 2.78 |
| $Pd_3Cu$@Pd | -1.15 | 0.92 | -1.72 | 1.40 | 0.31 | 3.95 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.13 | 2.78 |
| $Pd_3Zn$@Pd | -1.04 | 0.93 | -1.77 | 1.38 | 0.16 | 4.96 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.06 | 2.78 |
| $Pd_3Ga$@Pd | -1.15 | 0.93 | -1.85 | 1.48 | 0.06 | 6.81 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.11 | 2.78 |
| $Pd_3Ge$@Pd | -1.01 | 0.93 | -1.99 | 1.58 | -0.16 | 6.31 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.16 | 2.78 |
| $Pd_3Y$@Pd | -0.82 | 0.93 | -1.51 | 1.31 | 1.45 | 7.46 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 1.93 | 2.78 |
| $Pd_3Zr$@Pd | -0.89 | 0.93 | -2.17 | 1.51 | 1.09 | 5.32 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 1.97 | 2.78 |
| $Pd_3Nb$@Pd | -0.80 | 0.92 | -2.59 | 1.58 | 0.87 | 4.56 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.05 | 2.78 |
| $Pd_3Mo$@Pd | -0.94 | 0.92 | -2.36 | 1.56 | 0.64 | 4.07 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.19 | 2.78 |
| $Pd_3Rh$@Pd | -1.24 | 0.92 | -1.82 | 1.41 | 0.32 | 3.84 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.22 | 2.78 |
| $Pd_3Pd$@Pd | -1.28 | 0.92 | -1.67 | 1.36 | 0.23 | 3.93 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.20 | 2.78 |
| $Pd_3Ag$@Pd | -1.24 | 0.93 | -1.53 | 1.29 | 0.15 | 4.68 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.14 | 2.78 |
| $Pd_3In$@Pd | -1.14 | 0.93 | -1.66 | 1.39 | -0.47 | 13.27 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.10 | 2.78 |
| $Pd_3Sn$@Pd | -1.02 | 0.93 | -1.79 | 1.43 | 0.11 | 6.88 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.14 | 2.78 |
| $Pd_3La$@Pd | -0.80 | 0.93 | -1.48 | 1.25 | 1.59 | 8.21 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 1.89 | 2.78 |
| $Pd_3Ta$@Pd | -0.76 | 0.91 | -2.76 | 1.67 | 0.92 | 4.73 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.02 | 2.78 |

| | | | | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| $Pd_3W$@Pd | -0.83 | 0.91 | -2.67 | 1.68 | 0.71 | 4.16 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.23 | 2.78 |
| $Pd_3Re$@Pd | -0.93 | 0.92 | -2.45 | 1.65 | 0.47 | 3.74 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.13 | 2.78 |
| $Pd_3Os$@Pd | -1.08 | 0.92 | -2.20 | 1.59 | 0.32 | 3.61 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.20 | 2.78 |
| $Pd_3Ir$@Pd | -1.20 | 0.92 | -1.93 | 1.50 | 0.20 | 3.75 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.20 | 2.78 |
| $Pd_3Pt$@Pd | -1.31 | 0.92 | -1.72 | 1.42 | 0.13 | 3.96 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.22 | 2.78 |
| $Pd_3Au$@Pd | -1.34 | 0.93 | -1.54 | 1.35 | 0.02 | 4.63 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.27 | 2.78 |
| $Pd_3Tl$@Pd | -1.23 | 0.93 | -1.57 | 1.37 | -0.62 | 12.30 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.06 | 2.78 |
| $Pd_3Pb$@Pd | -1.04 | 0.93 | -1.59 | 1.33 | -0.11 | 9.09 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.23 | 2.78 |
| $Pd_3Bi$@Pd | -0.99 | 0.94 | -1.86 | 1.42 | -0.57 | 11.88 | 5.90 | 1.52 | 0.94 | 8.34 | 0.56 | 2.20 | 2.16 | 2.78 |
| $Pt_3Sc$@Pt | -1.23 | 0.89 | -2.00 | 1.83 | 0.69 | 4.14 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.03 | 3.90 |
| $Pt_3Ti$@Pt | -1.31 | 0.89 | -2.45 | 1.96 | 0.56 | 3.62 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.09 | 3.90 |
| $Pt_3V$@Pt | -1.37 | 0.88 | -2.47 | 1.98 | 0.47 | 3.49 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.12 | 3.90 |
| $Pt_3Cr$@Pt | -1.39 | 0.88 | -2.23 | 1.92 | 0.41 | 3.58 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.12 | 3.90 |
| $Pt_3Co$@Pt | -1.44 | 0.88 | -2.25 | 1.95 | 0.28 | 3.46 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.18 | 3.90 |
| $Pt_3Ni$@Pt | -1.51 | 0.88 | -2.16 | 1.91 | 0.28 | 3.50 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.19 | 3.90 |
| $Pt_3Cu$@Pt | -1.44 | 0.88 | -2.03 | 1.88 | 0.26 | 3.61 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.19 | 3.90 |
| $Pt_3Zn$@Pt | -1.38 | 0.89 | -2.03 | 1.86 | 0.21 | 4.10 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.12 | 3.90 |
| $Pt_3Ga$@Pt | -1.48 | 0.89 | -2.12 | 1.95 | 0.15 | 4.66 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.17 | 3.90 |
| $Pt_3Ge$@Pt | -1.52 | 0.89 | -2.29 | 2.01 | 0.03 | 4.67 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.22 | 3.90 |
| $Pt_3Y$@Pt | -1.24 | 0.89 | -1.71 | 1.68 | 0.91 | 5.10 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 1.98 | 3.90 |
| $Pt_3Zr$@Pt | -1.33 | 0.89 | -2.19 | 1.89 | 0.72 | 3.97 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.02 | 3.90 |
| $Pt_3Nb$@Pt | -1.20 | 0.88 | -2.59 | 2.01 | 0.61 | 3.61 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.11 | 3.90 |
| $Pt_3Mo$@Pt | -1.32 | 0.88 | -2.55 | 2.00 | 0.48 | 3.41 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.25 | 3.90 |
| $Pt_3Ru$@Pt | -1.57 | 0.88 | -2.22 | 1.91 | 0.28 | 3.39 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.26 | 3.90 |
| $Pt_3Rh$@Pt | -1.61 | 0.88 | -2.12 | 1.87 | 0.25 | 3.50 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.28 | 3.90 |
| $Pt_3Pd$@Pt | -1.65 | 0.88 | -1.97 | 1.81 | 0.22 | 3.60 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.26 | 3.90 |
| $Pt_3Ag$@Pt | -1.58 | 0.89 | -1.79 | 1.74 | 0.18 | 4.01 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.20 | 3.90 |
| $Pt_3In$@Pt | -1.45 | 0.89 | -1.89 | 1.81 | -0.17 | 7.59 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.16 | 3.90 |
| $Pt_3Sn$@Pt | -1.43 | 0.90 | -2.00 | 1.82 | 0.14 | 4.85 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.20 | 3.90 |
| $Pt_3La$@Pt | -1.25 | 0.90 | -1.56 | 1.54 | 0.96 | 5.53 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 1.94 | 3.90 |
| $Pt_3Ta$@Pt | -1.15 | 0.88 | -2.73 | 2.11 | 0.66 | 3.67 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.08 | 3.90 |
| $Pt_3W$@Pt | -1.18 | 0.87 | -2.72 | 2.13 | 0.51 | 3.38 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.30 | 3.90 |
| $Pt_3Re$@Pt | -1.38 | 0.87 | -2.58 | 2.10 | 0.35 | 3.26 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.19 | 3.90 |
| $Pt_3Os$@Pt | -1.51 | 0.88 | -2.40 | 2.03 | 0.27 | 3.33 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.26 | 3.90 |
| $Pt_3Ir$@Pt | -1.62 | 0.88 | -2.18 | 1.95 | 0.20 | 3.47 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.26 | 3.90 |
| $Pt_3Pt$@Pt | -1.70 | 0.88 | -2.03 | 1.87 | 0.17 | 3.65 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.28 | 3.90 |
| $Pt_3Au$@Pt | -1.72 | 0.89 | -1.80 | 1.77 | 0.13 | 4.01 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.34 | 3.90 |
| $Pt_3Tl$@Pt | -1.56 | 0.89 | -1.77 | 1.76 | -0.30 | 7.25 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.11 | 3.90 |
| $Pt_3Pb$@Pt | -1.43 | 0.90 | -1.81 | 1.69 | 0.02 | 5.88 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.29 | 3.90 |
| $Pt_3Bi$@Pt | -1.46 | 0.90 | -1.91 | 1.73 | -0.22 | 7.63 | 6.74 | 1.53 | 1.04 | 9.00 | 2.13 | 2.28 | 2.22 | 3.90 |

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