Effect of CO and H adsorption on the compositional structure of binary nanoalloys via DFT modelling

Supplementary Material

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Interaction energies per CO molecule ($E_i$) are calculated using the formula:

$$E_i = \frac{E_{\text{clust}} - E_{\text{bare}} - XE_{\text{CO}}}{X}$$

where $E_{\text{clust}}$ is the total energy of the cluster (both in absence and in presence of a $X$ number of CO molecules adsorbed), $E_{\text{bare}}$ is the energy of the cluster without molecules adsorbed on its surface and $E_{\text{CO}}$ is the energy of the CO molecule. This formula is given in explicit form for CO, but holds with appropriate modifications for adsorption of H atoms.

Figures S1 and S2 show the interaction energies as a function of the number of CO molecules and H atoms adsorbed on the AuPd, PdPt, CuPt and PdRh systems, respectively.

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Figure S1. Interaction energies per CO molecule (in eV) on the eight compositions investigated, as a function of the number of CO ligands attached to the surface. The blue lines refer to the cent configuration, the green ones to the core configuration and the red ones to the hex configuration.
Figure S2. Interaction energies per H atom (in eV) on the eight compositions investigated, as a function of the number of H ligands attached to the surface. The blue lines refer to the cent configuration, the green ones to the core configuration and the red ones to the hex configuration.