Supporting Information

A casting combined quenching strategy to prepare PdAg single atom alloy designed by Cluster Expansion combined Monte Carlo method

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We have calculated the frequency of CO-Pd bond using DFT simulation. The CO molecule adsorbed on Pd monomer (top site) and Pd dimer (bridge site) of PdAg(111) surface (see Figure 1), which compared with CO on top site and bridge site of pure Pd(111) surface (Table 1).

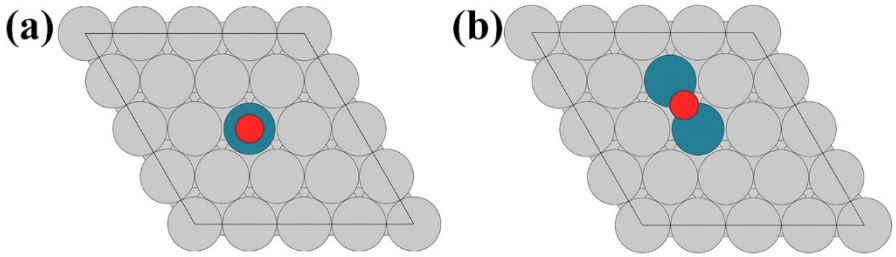

Figure 1. The CO adsorption positions on (a) Pd monomer (top site) and (b) Pd dimer (bridge site) of PdAg(111) surface. CO molecule, Ag atoms and Pd atoms are marked in red, grey and green, respectively.

Not only the trends of frequency changes on different surfaces but also the simulated value shows a good agreement with the experimental one. The linear CO frequency (top site) is about 100 cm^{-1} larger than bridge CO, which agree with the practical experience. The Pd-CO frequency on PdAg surface is lower than on pure Pd surface, which can be explained by the fact that the charge transfer from Ag to Pd increases the 2π back donation from Pd to the carbonyl C atom.

Table 1. The comparison of the frequency of CO-Pd bond between experiments and simulations

Frequency (cm^{-1})	Pd monomer (PdAg(111))	Pd dimer (PdAg(111))	Pure Pd surface (top site)	Pure Pd surface (bridge site)
Experiment	2023	1922	2108[1]	1925[1]
Simulation	2049	1903	2086[1]	1913[1]

References

[1] K. Honkala, P. Pirilä and K. Laasonen, CO and NO adsorption and co-adsorption on the Pd(111) surface, *Surf. Sci.*, 2001, 489, 72–82.