

Supplementary Table Captions

ST1: Binding energy (E_b) and related bond lengths of H_2 , H, 2H, CO_2 , HOCO, HCOO and HCOOH on Pd_4Cu_4 cluster.

ST2: Binding energy (E_b) and related bond lengths of H_2 , H, 2H, CO_2 , HOCO, HCOO and HCOOH on $Pd_{12}Cu$ cluster.

ST3: Geometric isomers of Pd_4 , Pd_mCu_n ($m+n = 4$) and Cu_4 clusters (Atomic colours: Green = Pd, Brown= Cu)

ST4: Geometric isomers of Pd_8 , Pd_mCu_n ($m+n = 8$) and Cu_8 clusters (Atomic colours: Green = Pd, Brown= Cu)

ST5: Geometric isomers of $CuPd_{12}$ cluster (Atomic colours: Green = Pd, Brown= Cu)

ST6: Total Charge distribution ($e/\text{Å}^3$) on atoms of Pd_2Cu_2 and CO_2 adsorbed Pd_2Cu_2 cluster ($Pd_2Cu_2-CO_2$).

ST7: Total Charge distribution ($e/\text{Å}^3$) on atoms of Pd_4Cu_4 and CO_2 adsorbed Pd_4Cu_4 cluster ($Pd_4Cu_4-CO_2$).

ST8: Total Charge distribution ($e/\text{Å}^3$) on atoms of $Pd_{12}Cu$ and CO_2 adsorbed $Pd_{12}Cu$ cluster ($Pd_{12}Cu-CO_2$).

ST9: Lowest energy Pd_4 , Cu_4 , Pd_8 , Cu_8 and Pd_mCu_n ($m+n=4, 8$ and 13) clusters along with their position coordinates (in cartesian). (Atomic colours: Green: Pd, Brown: Cu)

Supplementary Figure Captions

SF1: Lowest energy structure of Pd₄Cu₄ clusters along with their (a) H₂ (b) H (c) 2H (d) CO₂ (e) CO₂+H (f) Carboxyl (g) HCOO (h) HCOO+H and (i) HCOOH adsorbed species.

SF2: Lowest energy structure of Pd₁₂Cu clusters along with their a) H₂ (b) H (c) 2H (d) CO₂ (e) CO₂+H (f) Carboxyl (g) HCOO (h) HCOO+H and (i) HCOOH adsorbed species.

SF3: The potential energy profile for the formation of (a) bidentate formate by the reaction of H-atom and CO₂ (b) formic acid by the reaction of H-atom and formate on Pd₄Cu₄ cluster.

SF4: The potential energy profile for the formation of (a) bidentate formate by the reaction of H-atom and CO₂ (b) formic acid by the reaction of H-atom and formate on Pd₁₂Cu cluster.

SF5(a): Total density of states of Pd₂Cu₂ cluster along with Pd and Cu in that cluster.

SF5(b): The orbital projected density of states of Pd₂Cu₂ cluster.

SF6(a): Total density of states of Pd₂Cu₂_CO₂ cluster along with its constituent elements.

SF6(b): The orbital projected density of states of Pd₂Cu₂_CO₂ cluster.