

Supplementary Information

**Correlating binding energies of adsorbed CO and H on model surfaces with CO/H₂ selectivity from
co-electrolysis of CO₂ and H₂O over copper-palladium bimetallic catalysts**

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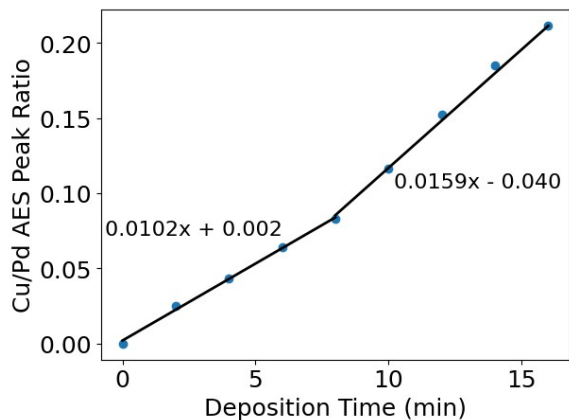


Figure S1. AES peak ratios for Cu (920 eV)/Pd(270 eV) as a function of deposition time. After 8 minutes, a change in the slope indicated the formation of 1 ML of Cu on the Pd(111) surface.

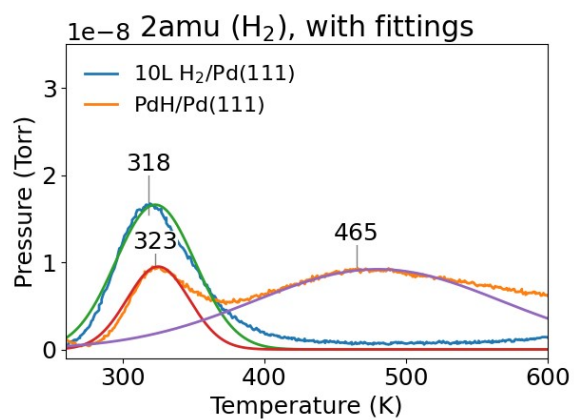


Figure S2. Gaussian fitting overlaid over the H₂ TPD spectra from Pd(111) and PdH/Pd(111).

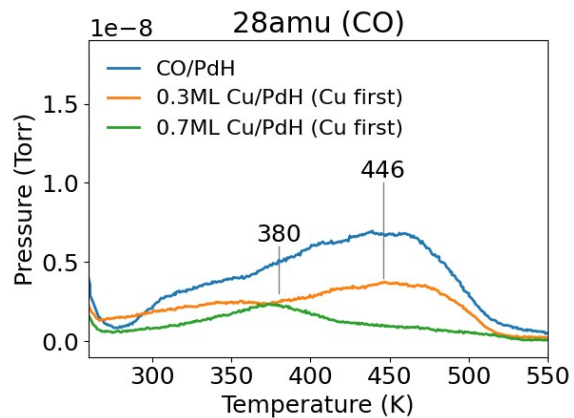


Figure S3. TPD spectra of CO desorption from Cu/Pd(111) surfaces that had Cu deposited first and then was subsequently treated with 600L H_2 to form a bulk Cu/PdH phase.

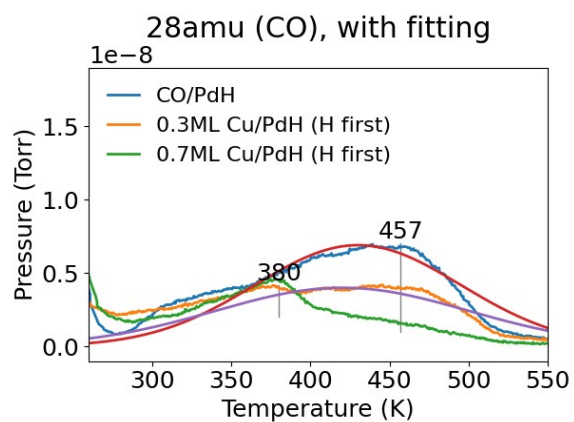


Figure S4. Gaussian fitting overlaid over the CO TPD spectra from Cu/Pd(111) and Cu/PdH surfaces.

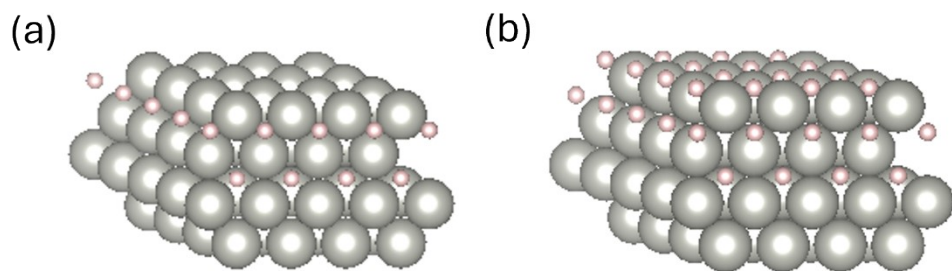


Figure S5. (a) Pd-terminated PdH(111) and (b) H-terminated PdH(111). (Grey: Pd; Pink: H)

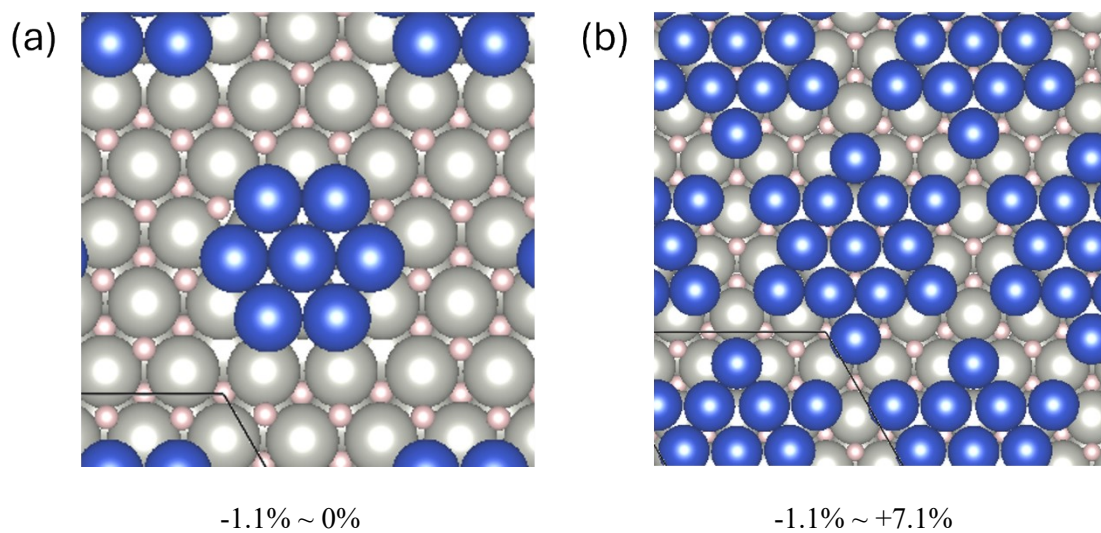


Figure S6. Determination of (a) 0.3ML Cu/PdH and (b) 0.7ML Cu/PdH structure with lowest energy and Cu-Cu bond strain range. (Grey: Pd; Blue: Cu; Pink: H)

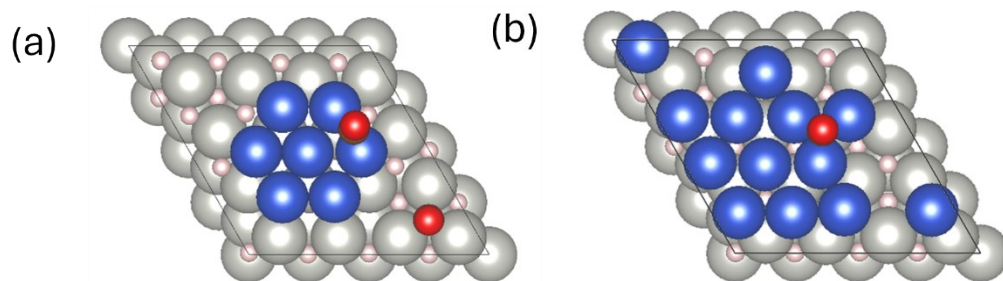


Figure S7. Most stable CO binding site on (a) 0.3ML Cu/PdH (Cu site B.E. = -1.10eV, Pd site B.E. = -1.27eV); (b) 0.7ML Cu/PdH (-1.17eV). (Grey: Pd; Blue: Cu; Pink: H; Red: CO)