Electronic Supplementary Information

Unveiling CO adsorption on Cu Surfaces: New Insights from Molecular Orbital Principles

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The adsorption energy data from literature presented in Tables S1 and S2 below are specifically for CO adsorption on Cu surfaces at low (Θ= ¼) monolayer coverage. The system that is most frequently studied theoretically, at the specified coverage, is the CO adsorption Cu(111). A fewer theoretical studies for CO adsorption on Cu(100) are available in literature. However, only one theoretical study that included a value for CO (Θ= ¼ ML coverage) adsorption on Cu(110) is available in the literature with a value of -0.94 eV at the ontop-site calculated using GGA PBE functional.

Table S1: The reported adsorption energies for CO on Cu (111) surfaces in the literature.

Cu (111)	PW91	RPBE	PBE	LDA	PBEsol	BLYP	PBE0	HSE03
Top	-0.72[ref 1] -0.73[ref 2] -0.75[ref 3] -0.77[ref 4]	-0.42[ref 1] -0.42[ref 2] -0.38[ref 3] -0.48[ref 4]	-0.75[ref 5] -0.71[ref 6] -0.74[ref 7]	-1.29[ref 6]	-1.05[ref 7]	-0.27[ref 7]	-0.61[ref 6]	-0.56[ref 6]
Bridge	-0.74[ref 2] -0.83[ref 3] -0.80[ref 4]	-0.39[ref 2] -0.39[ref 3] -0.46[ref 4]	-0.82[ref 5]	-1.86[ref 8]				
Hollow fcc	-0.84[ref 2] -0.91[ref 3] -0.87[ref 4]	-0.46[ref 2] -0.44 [ref 3] -0.50[ref 4]	-0.87[ref 6] -0.80[ref 7]	-1.66[ref 6]	-1.23[ref 7]	-0.34[ref 7]	-0.58[ref 6]	-0.56[ref 6]
Hollow hcp	-0.83[ref 2] 0.89[ref 3] -0.86[ref 4]	-0.45[ref 2] -0.43[ref 3] -0.49[ref 4]	-0.89[ref 5] -0.86[ref 6]	-1.64[ref 6]			-0.57[ref 6]	-0.54[ref 6]

Table S2: The reported adsorption energies for CO on Cu (100) surfaces in the literature

Cu (100)	PW91	RPBE
Top	-0.863[ref 2]	-0.565[ref 2]
Bridge	-0.883[ref 2]	-0.545[ref 2]
Hollow	-0.842[ref 2]	-0.471[ref 2]

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