

First-principles descriptors of CO chemisorption on Ni and Cu surfaces
Supporting Information

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1. Copper Mulliken's Charge Transfer Tables:

Positive indicates electron gain and negative indicates electrons lost.

Cu	100			110				111			
	Top	Bridge	Hollow	Top	Short Bridge	Long Bridge	Hollow	Top	Bridge	FCC	HCP
s	-0.29	-0.28	-0.32	-0.14	-0.16	-0.22	-0.36	-0.23	-0.29	-0.32	-0.33
p	0.33	0.16	0.10	0.12	0.04	-0.02	0.06	0.21	0.11	0.09	0.07
d	-0.15	-0.18	-0.22	-0.09	-0.18	-0.11	-0.14	-0.09	-0.12	-0.14	-0.11

2. Nickel Mulliken's Charge Transfer Tables:

Positive indicates electron gain and negative indicates electrons lost.

Ni	100			110				111			
	Top	Bridge	Hollow	Top	Short Bridge	Long Bridge	Hollow	Top	Bridge	FCC	HCP
s	-0.22	-0.30	-0.39	-0.11	-0.18	-0.42	-0.39	-0.16	-0.25	-0.27	-0.28
p	-0.02	-0.21	-0.30	-0.05	-0.18	-0.20	-0.13	0.06	-0.08	-0.12	-0.14
d	0.07	0.14	0.14	-0.07	-0.02	0.04	0.0	-0.04	-0.02	0.03	-0.01