

Supporting Information:

In search of non-conventional surface oxidic motifs of Cu on Au(111)

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TABLE S1. Average adsorption energies of oxygen in various oxidic structures (i.e. O/Cu(111),^{1,2} O/Au(111),³ and O/Cu on Au(111) at the corresponding surface oxygen coverage, Θ_{O} .

System	Oxidic structures	Θ_{O} (ML)	E^{ad} (eV/O atom)
Cu-O/Au(111)	<i>p2</i>	0.500	-1.94
	<i>p2</i> +Cu _F	0.500	-1.72
	<i>p2</i> +O _F	0.750	-1.28
	<i>p2s</i>	0.500	-1.96
	<i>p2s</i> +Cu _F	0.500	-1.77
	<i>p2s</i> +Cu _F -O _L	0.417	-1.73
	<i>p2s</i> -O _L	0.417	-1.86
	<i>p2(6q6)</i>	0.316	-1.86
	<i>p2(6q6)</i> +O ₃	0.474	-1.79
	<i>p2(6q6)</i> -Cu ₃	0.316	-1.86
	<i>p2(6q6)</i> -Cu ₆	0.316	-1.59
	<i>p4</i>	0.375	-1.62
	<i>p4</i> +O _F	0.438	-1.46
	<i>p4</i> +O _{HF}	0.500	-1.28
	<i>p4</i> +O _{BBB}	0.563	-1.14
	<i>p4</i> -OCu ₃	0.313	-1.81
	O/Cu(111) ¹	<i>p2</i>	0.500
<i>p2</i> +Cu _F		0.500	-1.68
<i>p2</i> +O _F		0.750	-1.77
<i>p4</i>		0.375	-2.14
<i>p4</i> +Cu _T		0.375	-1.99
<i>p4</i> +Cu _H		0.375	-2.10
<i>p4</i> +Cu _{FH}		0.375	-2.04
<i>p4</i> +Cu _{HT}		0.375	-1.93
<i>p4</i> +Cu _T +O _F		0.438	-1.99
<i>p4</i> +O _F		0.438	-2.10
<i>p4</i> +O _H		0.438	-2.09
<i>p4</i> +O _{FH}		0.500	-2.05
<i>p4</i> -OCu ₃		0.313	-2.15
<i>p4</i> -(OCu ₃) ₂		0.250	-2.09
“8”-structure ²		0.500	-1.79
O/Au(111) ³		0.063	-0.75
		0.111	-0.66
	Chemisorbed	0.250	-0.64
	overlayers	0.500	-0.30
		0.750	0.16
	1.000	0.62	

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