Supporting Information:

Ab Initio Thermodynamics of Surface Oxide Structures Under Controlled Growth Conditions

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Table S1: The computed the change of Cu chemical potential ($\Delta\mu_{\mathrm{Cu}}$) values for various structural models

Nano-composite	Θ_{Cu}	$\Delta\mu_{\mathrm{Cu}}$ (eV)
Bulk Cu	∞	-3.52
Cu monolayer	2.75	-3.06
	2.63	-3.12
	1.75	-2.92
Cu overlayer	1.00	-2.37
	0.38	-0.91
	0.36	-0.74
	0.33	-0.53
	0.28	-0.63
	0.25	0.12
	0.11	3.40
Surface alloy	0.75	-2.20
	0.50	-1.78
	0.33	-1.16
	0.25	-0.48
	0.11	2.95
Subsurface alloy	0.75	-2.89
	0.50	-2.43
	0.33	-1.79
	0.25	-1.06
	0.11	2.38

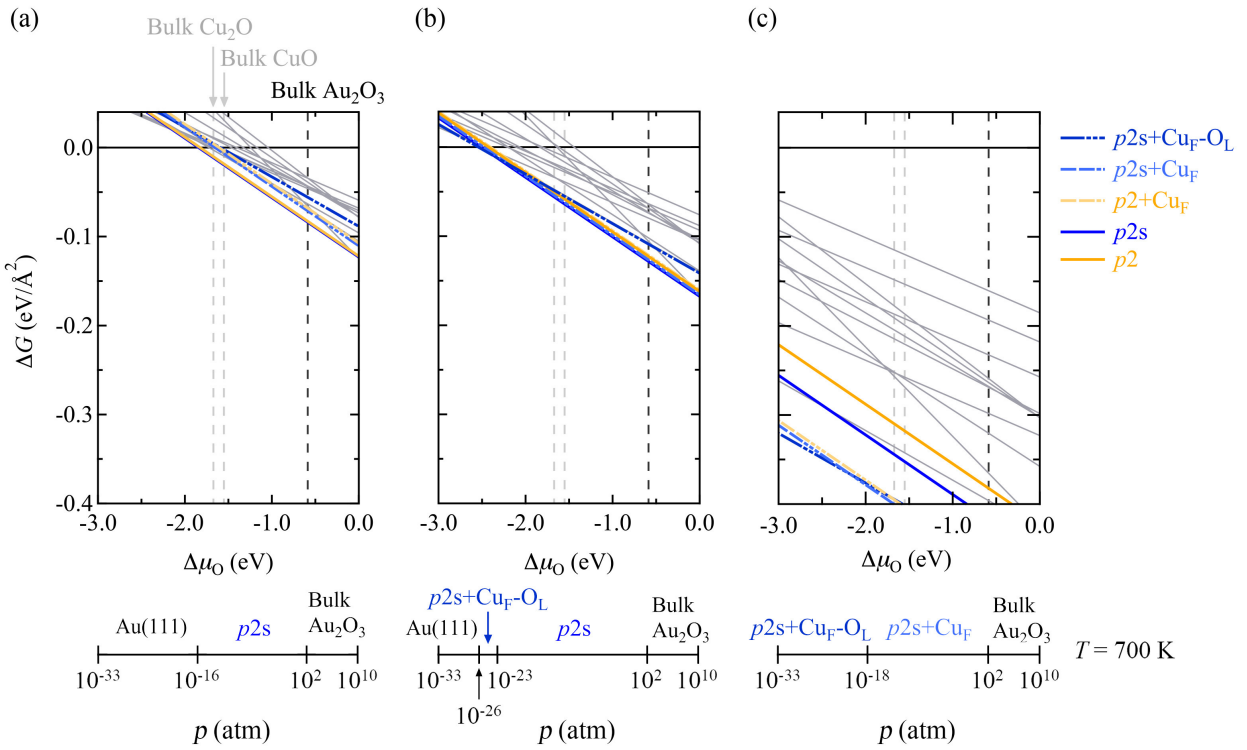

Figure S1: Calculated Gibbs free energy of adsorption, ΔG for various thin film oxides of Cu on Au(111) as a function of the change in oxygen chemical potential at specific $\Delta\mu_{Cu}$ values; (a) -3.52 eV which corresponds to bulk Cu, (b) -3.12 eV which corresponds to Θ_{Cu} = 2.63 ML, as an example of monolayer Cu_xAu_y structures, and (c) -0.53 eV which then corresponds to $\Theta_{Cu} = 0.33$ ML, as an example of overlayer Cu_xAu_y structures.