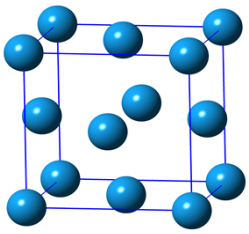
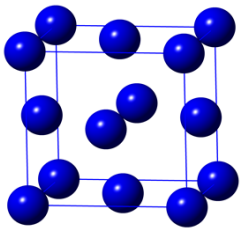
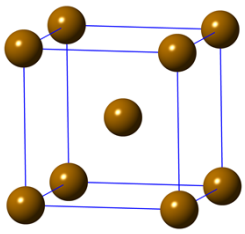
Supporting Information

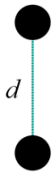
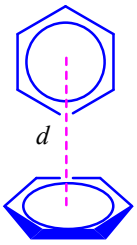
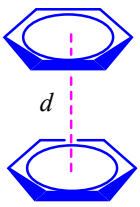
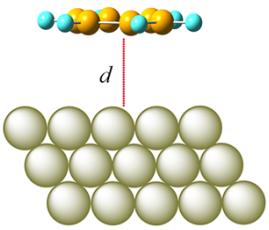
Some solids and molecular systems were investigated using DMol^3/GGA-PW91-OBS (λ = 3.0 × 10^{-5}, n = 8.0). The results are presented in Table S1~S2. They are compared with other theoretical data and available experimental findings. These survey results indicate that the proposed calculation parameter is acceptable.

Table S1 Calculated lattice constant a_0 for Al, Cu, and Fe crystals.

		Al	Cu	Fe
structure				
a_0 (Å)	calc.	4.042	3.645	2.846
	expt.	4.049[a]	3.614[b]	2.866[c]

[a] Ref. [1].
[b] Ref. [2].
[c] Ref. [3].

Table S2 Equilibrium distances d and binding energies E for neon, argon, benzene dimers, and benzene@Cu(111).

		rare-gas		benzene dimers		benzene@Cu(111)
		Ne_2	Ar_2	T-shaped	sandwich	
structure						
d (Å)	calc.	3.010	3.812	5.078	4.025 (3.900[e])	3.250
	expt.	3.094[a]	3.761[b]	4.960[d]		
E (eV)	calc.	0.013 (0.016[c])	0.012	0.123 (0.119[e])	0.084 (0.079[e])	0.520
	expt.	0.007[a]	0.024[b]			0.600[f]

[a] Ref. [4].
[b] Ref. [5].
[c] Ref. [6].
[d] Ref. [7].
[e] Ref. [8].
[f] Ref. [9, 10].

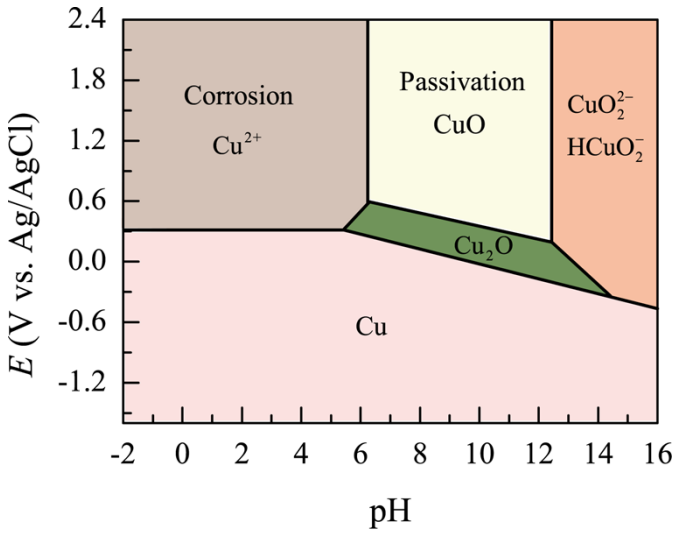


Fig. S Potential-pH equilibrium diagram for the system, copper–water, at 298 K.[11]

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