Electronic Supplementary Material (ESI) for Faraday Discussions.

Density functional theory based computational investigations on the stability of highly active trimetallic PtPdCu nanoalloys for electrochemical oxygen reduction

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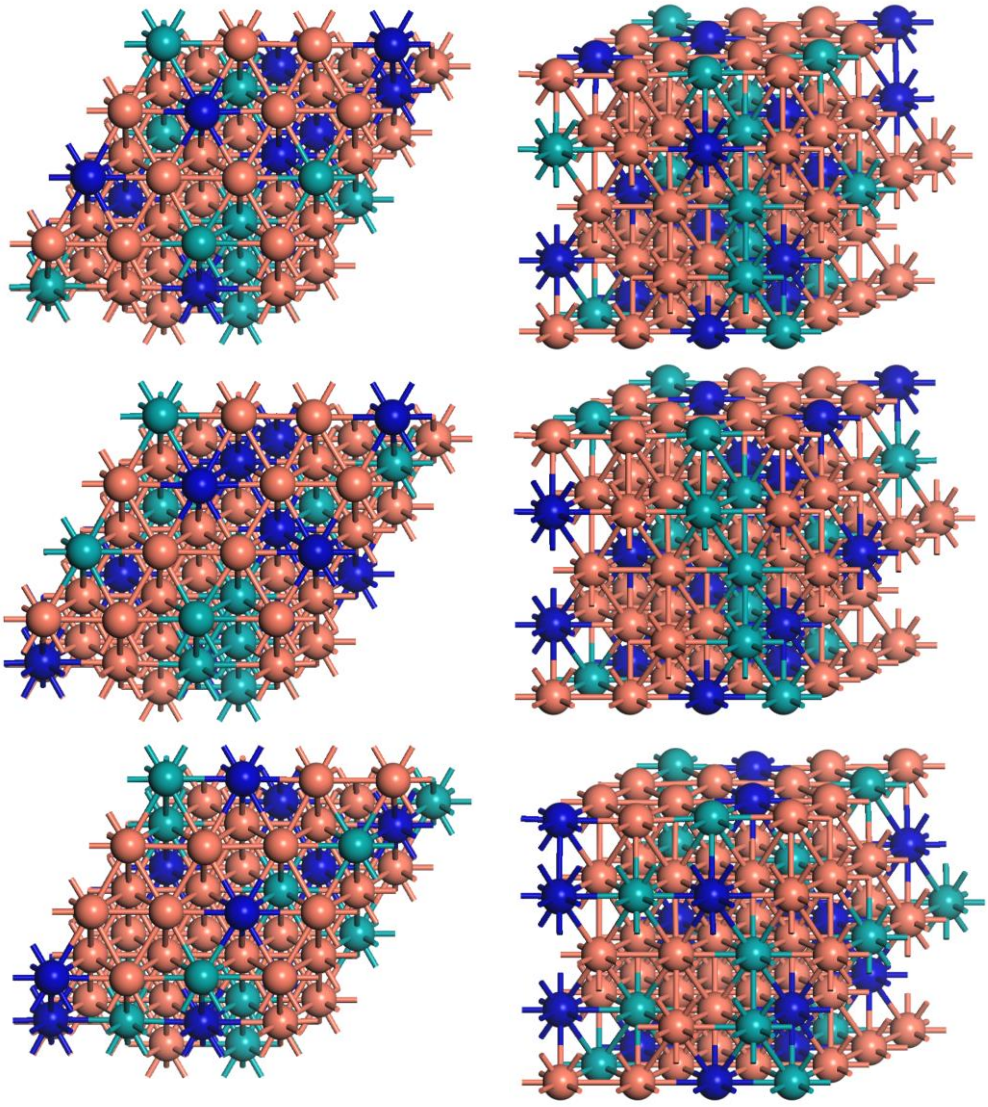

Fig. S1 The top view (left) and side view (right) of the model catalysts. Dark blue, blue, and brown balls represent Pt, Pd, and Cu atoms, respectively. The energy difference among the three model catalysts is less than 0.00009 eV/atom.

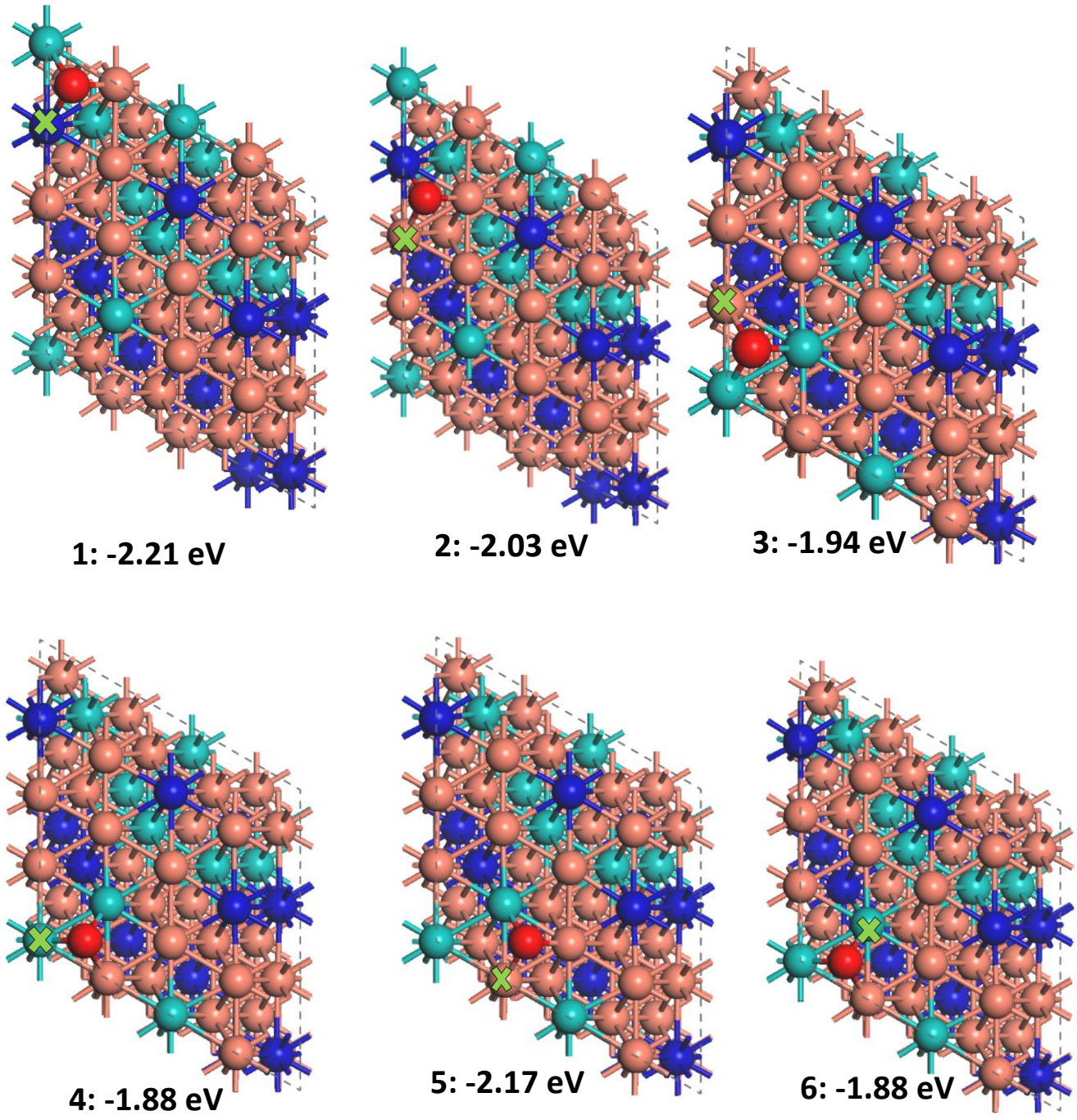

Fig. S2 Six DFT calculated configurations and energies of O adsorption on the model catalyst surface. Dark blue, blue, and brown balls represent Pt, Pd, and Cu atoms, respectively. The initial O was placed above of the atom marked by green X by 2.5 A.

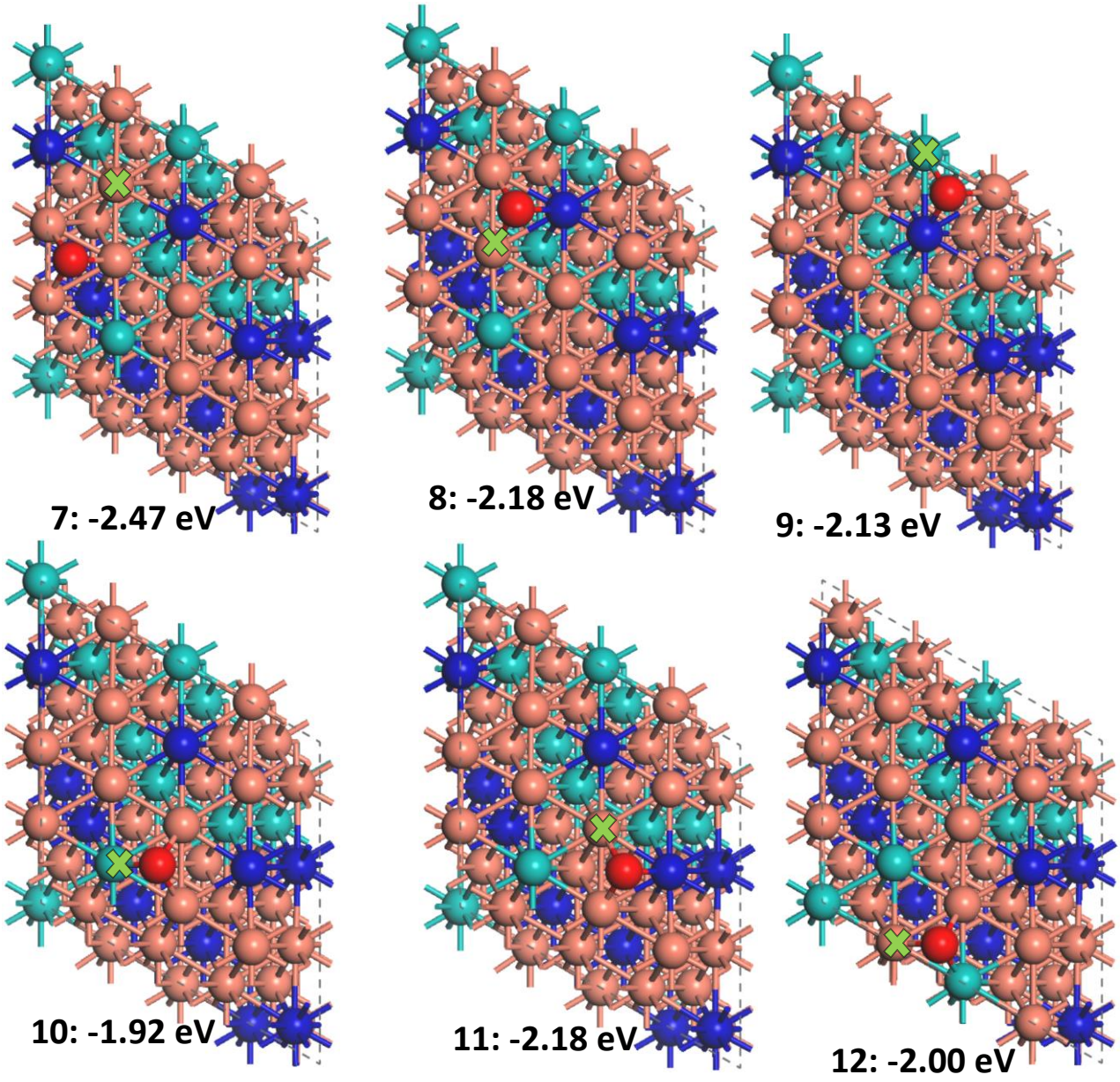

Fig. S3 Six DFT calculated configurations and energies of O adsorption on the model catalyst surface. Dark blue, blue, and brown balls represent Pt, Pd, and Cu atoms, respectively. The initial O was placed above of the atom marked by green X by 2.5 A.

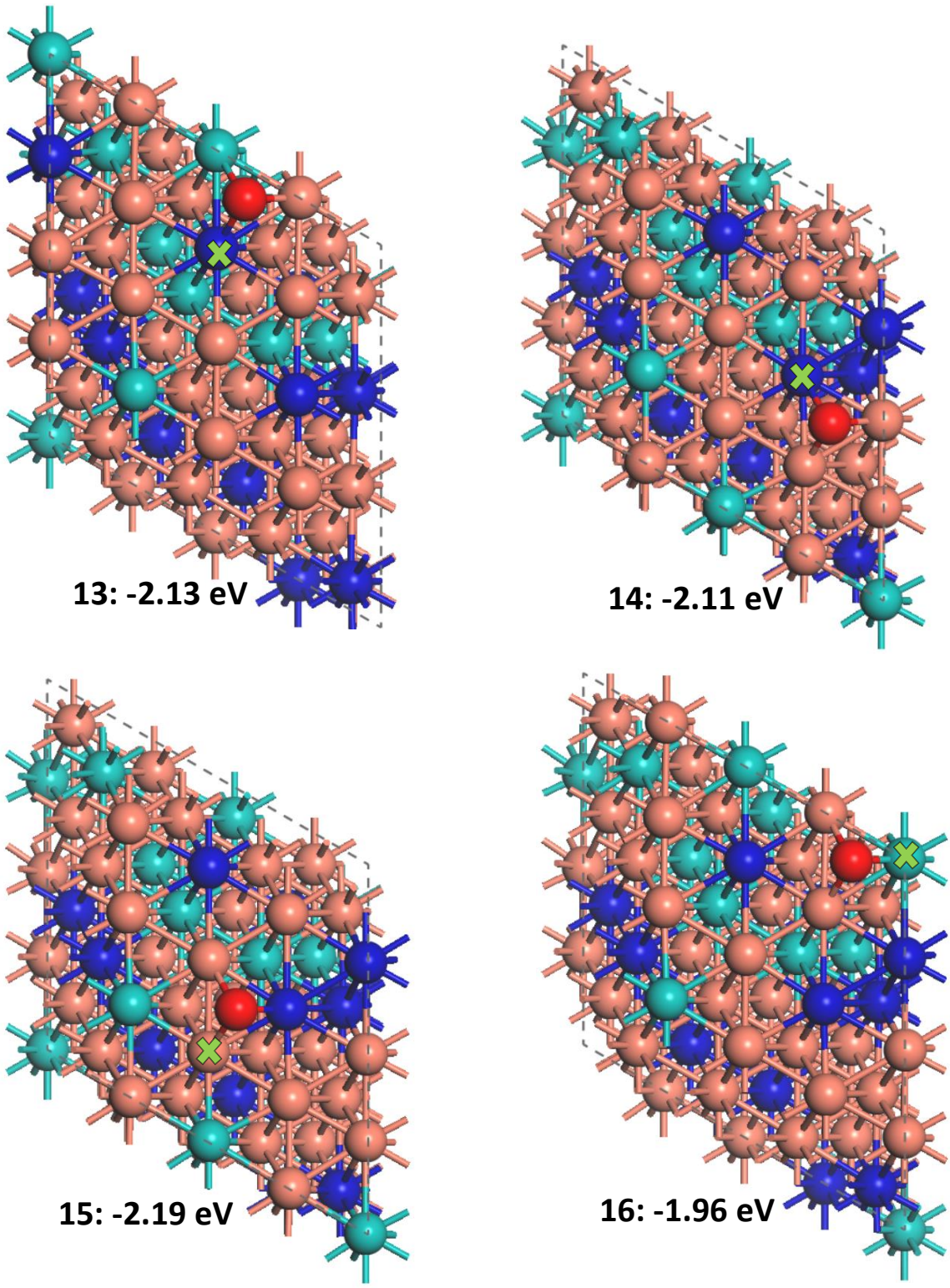

Fig. S4 Four DFT calculated configurations and energies of O adsorption on the model catalyst surface. Dark blue, blue, and brown balls represent Pt, Pd, and Cu atoms, respectively. The initial O was placed above of the atom marked by green X by 2.5 A.

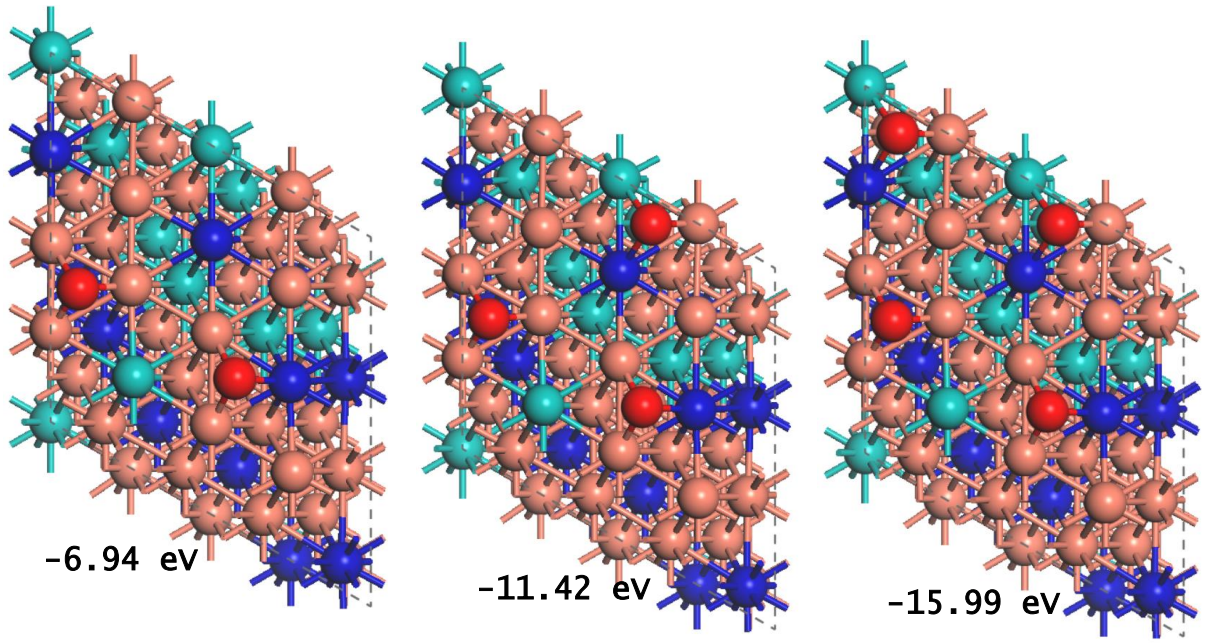

Fig. S5 DFT calculated configurations and energies of 2 O, 3 O, and 4 O adsorption on the model catalyst surface. Dark blue, blue, and brown balls represent Pt, Pd, and Cu atoms, respectively.

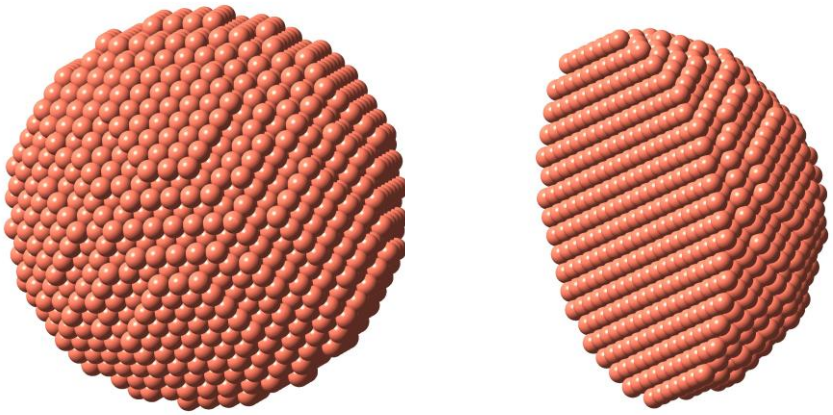

Fig. S6 Illustration of a 5.0 nm Cu particle of 5089 atoms: entire particle (left) and half size (right).

Table S1. The parameters calculating the rate constants at T=298K and U=0.9V

i	ΔG_i (eV)	A_i
1	0.7925[a]	1
2	0.968	1
3	0.6-0.5ΔE*	10^{13}
4	0.6+0.5ΔE*	10^{13}

[a] $\Delta G=(1-\beta)n(U-\phi^0)$,[1] where $\beta=0.29$, $n=2$, $U=0.9V$, $\phi^0=0.3419V$

*ΔE is a function of surface Cu composition and the values are shown in Fig. 5.

Reference

1. J. Zhu, S. Hu, Z. Zeng and W.-X. Li, J. Chem. Phys., 2019, 151, 234711.