

Supporting information for:

Water adsorption at the (010) and (101) surfaces of CuWO_4

Xuan Chu,¹ David Santos-Carballal,^{1,*} Nora H de Leeuw^{1,2}

¹School of Chemistry, University of Leeds, Leeds LS2 9JT, United Kingdom

²Department of Earth Sciences, Utrecht University, Princetonplein 8A, 3584 CD Utrecht, The Netherlands

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- Table S1. Adsorption energy calculated by DFT at 0 K (ΔE_{DFT}), Zero-point energy (ΔE_{zpe}), vibrational contribution to the entropy (ΔS), and Helmholtz free energy (ΔF) of pristine (010) and reduced (101) surface.

Configuration	ΔE_{DFT} (eV)	ΔE_{zpe} (eV)	ΔS (J/(mol·K))	ΔF (eV)
Pristine (010) surface				
$\mu_{3-\eta}^3$	-0.89	0.09	0.00012	-0.84
$\mu_{2-\eta}^2$	-0.69	0.09	0.00012	-0.64
$\mu_{1-\eta}^1$	-0.69	0.09	0.00012	-0.64
$\mu_{2-\eta}^2$	-0.26	0.09	0.00011	-0.21
$\mu_{2-\eta}^2$	-0.12	0.08	0.00015	-0.09
Reduced (101) surface				
$\mu_{2-\eta}^2$	-0.81	0.09	0.00012	-0.76
$\mu_{2-\eta}^2$	-0.63	0.09	0.00012	-0.58
$\mu_{3-\eta}^3$	-0.53	0.08	0.00012	-0.48
$\mu_{3-\eta}^3$	-0.53	0.08	0.00016	-0.50

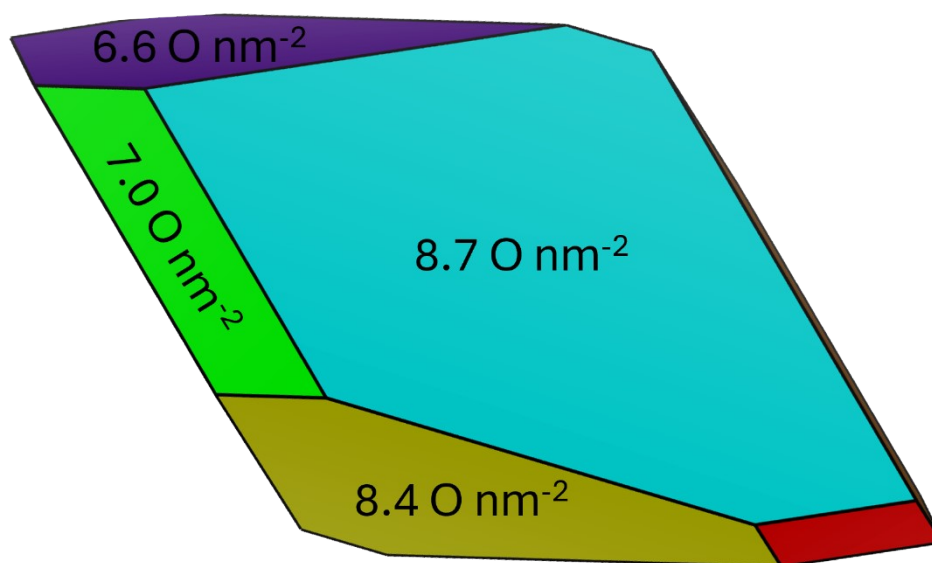


Figure S1. The equilibrium morphologies of CuWO_4 under 700 K. The pristine (001), oxidized (011), oxidized (100), oxidized (110), and oxidized (111) surfaces are coloured in red, yellow, green, cyan, and purple, respectively. The surface coverage of each surface is noted in the figure.