Supplementary Information

Cu(II) sorption by biogenic birnessite produced by *Pseudomonas putida* strain MnB1: Structural differences from abiotic birnessite and its environmental implications

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TABLES

Table S1. Mn 2p 3/2 fitting parameters obtained from Mn(IV), Mn(III) and Mn(II) multiplet peak fitting for abio- and bio-birnessite samples

		Abio-birnessite	Bio-birnessite
Mn(IV)	Binding energy* (eV)	642.3	642.0
	FWHM† (eV)	2.75	3.00
	Proportion‡ (%)	77.8	92.6
Mn(III)	Binding energy (eV)	641.5	641.5
	FWHM (eV)	1.40	0.80
	Proportion (%)	22.2	4.9
Mn(II)	Binding energy (eV)	-	640.5
	FWHM (eV)	-	0.80
	Proportion (%)	0	2.5

* The binding energy is constrained during fitting, as 641.9-642.6 eV for Mn(IV), 641.2-641.7 eV for Mn(III) and 640.0-640.9 eV for Mn(II).

† Full width at half maxima (constrained during fitting). All peaks modeled as Gaussian-Lorentzian = 50: 50.

‡ The area contribution of each peak under the Mn $2p_{3/2}$ peak.

FIGURES

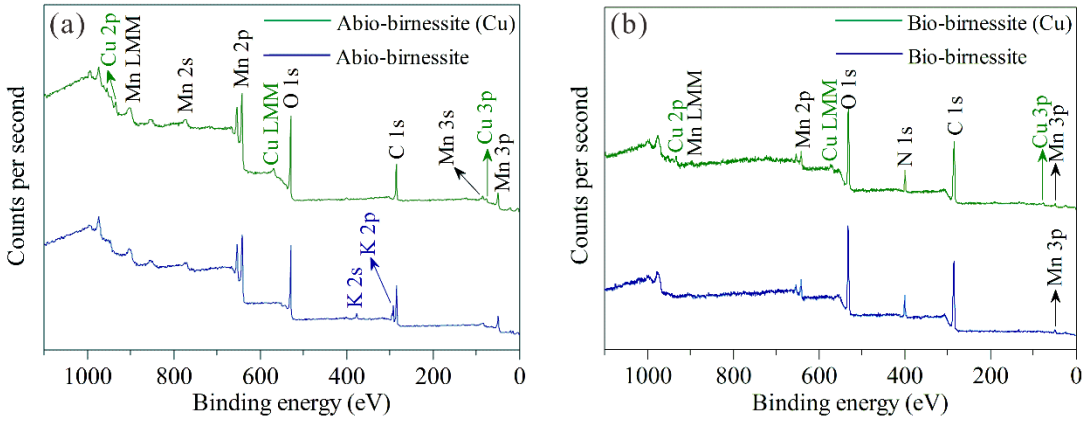

Fig. S1 XPS survey scans (broad scans) of (**a**) abio-birnessite and (**b**) bio-birnessite samples, both before and after Cu(II) adsorption. Texts in black indicate the photoelectron lines present on both raw and Cu(II)-adsorbed birnessite samples, while texts in green and blue refer to those distinguishable from each other.

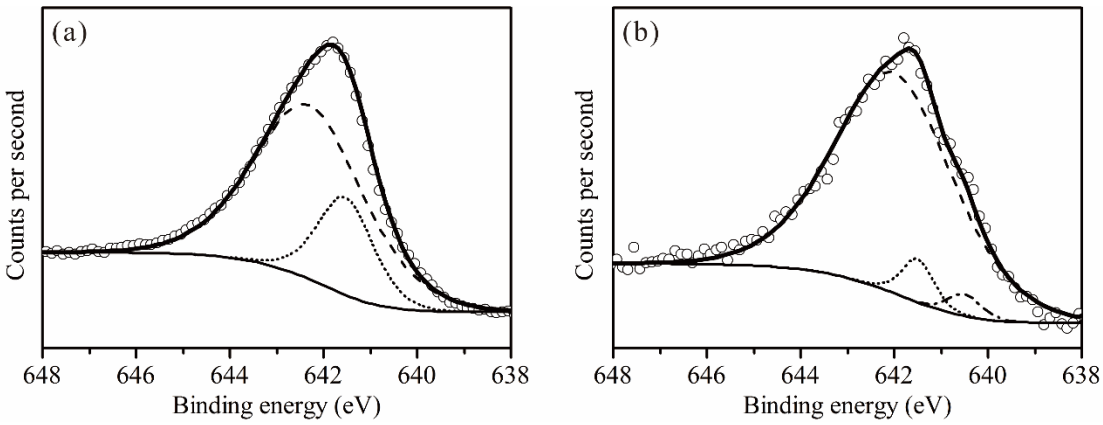

Fig. S2 XPS narrow scans of Mn $2p_{3/2}$ spectra (circle symbols) for (**a**) abio-birnessite and (**b**) bio-birnessite samples, plotted with the best fits (thick solid lines) as presented in **Table S1**. Deconvoluted peak fittings are conducted with Mn(IV) (dashed lines), Mn(III) (dotted lines), Mn(II) (dash-dotted lines) multiplet peaks and Shirley background (thin solid lines).

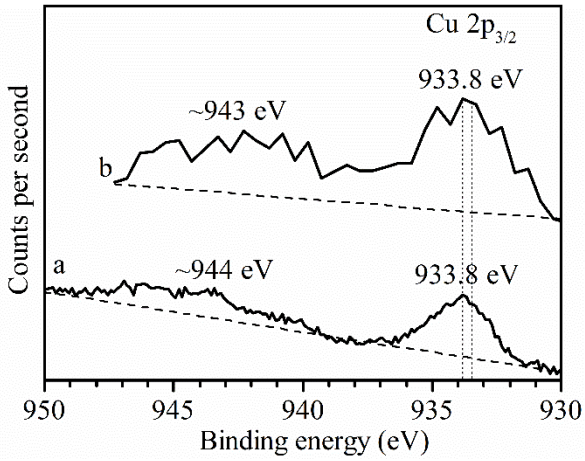

Fig. S3 XPS spectra of Cu $2p_{3/2}$ for Cu(II)-adsorbed abio-birnessite (**a**) and bio-birnessite (**b**). Both spectra display a peak maxima at 933.8 eV and a shake-up satellite at ~943-944 eV (~9 eV higher from the main peak), confirming the presence of Cu(II). Dashed lines are the linear baselines. (Notes: the spectrum of bio-birnessite is obtained from the survey scans and thus has larger energy size and fewer data points; yet still the broad shake-up satellite can be recognized, and the peak maxima can be positioned within 933.4-933.9 eV as indicated by the dotted vertical lines)