Supplementary materials for

Molecular mechanisms of dimethylarsinic acid adsorption onto aluminum substituted ferrihydrite surfaces

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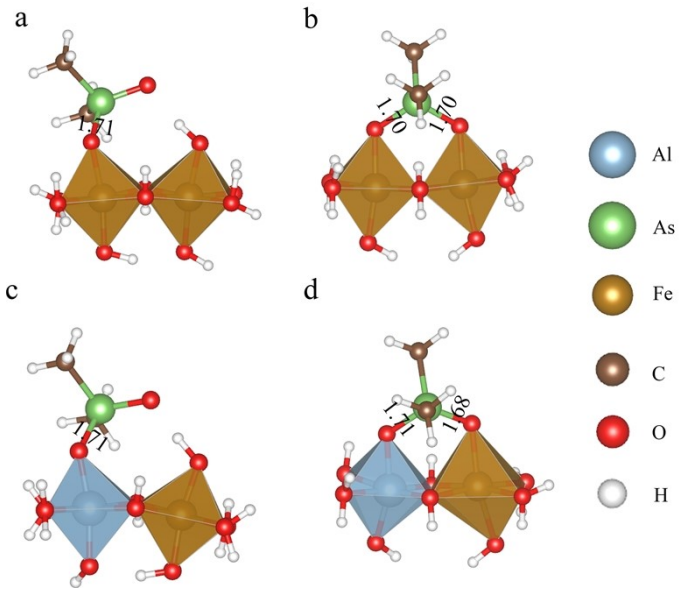

Figure S1 The geometry optimized structures of DMA binding to edge-sharing dioctahedral cluster $Fe_2(OH)_6 \cdot 4H_2O$ or $Fe(OH)_3Al(OH)_3 \cdot 4H_2O$.

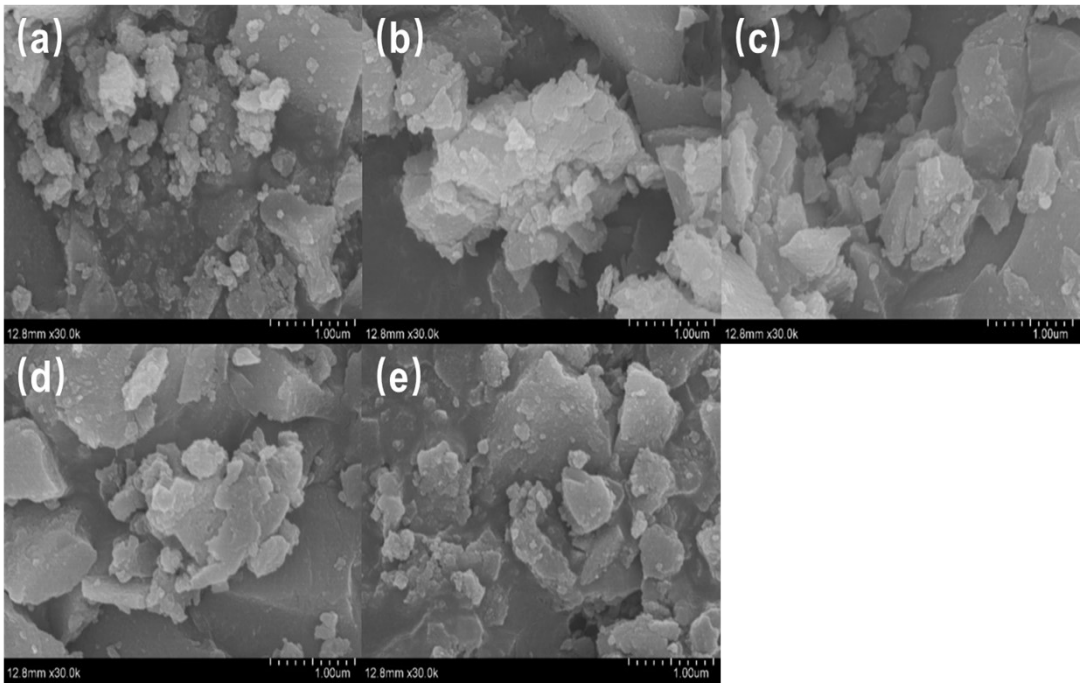

Figure S2 FESEM images of Al-substituted ferrihydrite samples.

(a) Fh, (b) FhAl0.05, (c) FhAl0.1,(d) FhAl0.2, and (e) FhAl0.3

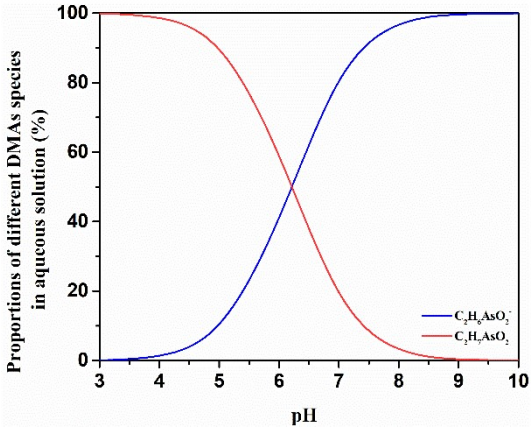

Figure S3 Proportions of various DMAs species as a function of pH. The dissociation constant of DMAs (pK_a) is 6.2.[1]

Table S1 Langmuir fitting parameters of DMAs adsorption isothermal curves on Al-substituted ferrihydrite samples.

Sample	Q_m (μmol·m^{-2})	affinity constant (L·μmol^{-1})	R^2
Fh_W	1.77	0.08±0.01	0.9878
Fh	1.85	0.01±0.00	0.9949
FhAl0.05	2.84	0.05±0.01	0.9949
FhAl 0.1	2.98	0.05±0.01	0.9936
FhAl0.2	2.74	0.03±0.00	0.9949
FhAl0.3	2.70	0.03±0.01	0.9831

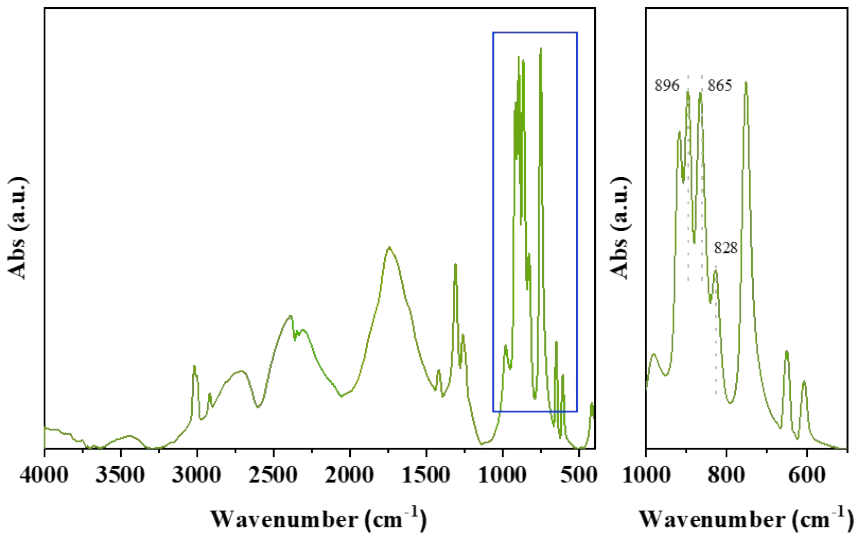

Figure S4 FTIR spectra of DMAs from 400-4000 cm^{-1} (left) and 500-1000 cm^{-1} (right).

References

1. B. J. Lafferty and R. H. Loeppert, Methyl arsenic adsorption and desorption behavior on iron oxides, Environ Sci Technol, 2005, 39, 2120–2127.