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Supplement of

Surface complexation modeling of Cd(II) sorption to montmorillonite, bacteria, and their composite

Ning Wang et al.

Correspondence to: Q. Huang (qyhuang@mail.hzau.edu.cn) and W. Chen (wlchen@mail.hzau.edu.cn)

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Determination of SSA in aqueous.

According to the Tournassat et al. (2003), the specific surface area (SSA) of clay minerals measured by BET is recognized as the basal surface area + edge surface area. However, a particle is supposed to form nearly 20 stacked layers in the dehydrated state during the gas adsorption experiment, whereas it is estimated to be composed of only 1 or 2 layers in aqueous suspension. Herein in our experiments, this “interlayer surface area” must be taken into account. According to the estimation of Tournassat et al. (2003), the basal, interlayer, edge and total surface area of a Na-MX80 clay is 26.6, 753, 8.5 and 788 m^2/g, respectively. The basal + edge surface area for the montmorillonite used in this study is 60.2 m^2/g. If we assume the “interlayer surface area” is 753 m^2/g, the total surface area in aqueous phase should be ~813 m^2/g. Therefore we set the SSA to be 800 m^2/g in this study. In comparison to the values obtained from gas adsorption method, this value may reflect, to a large extent, the realistic situation in aqueous system.

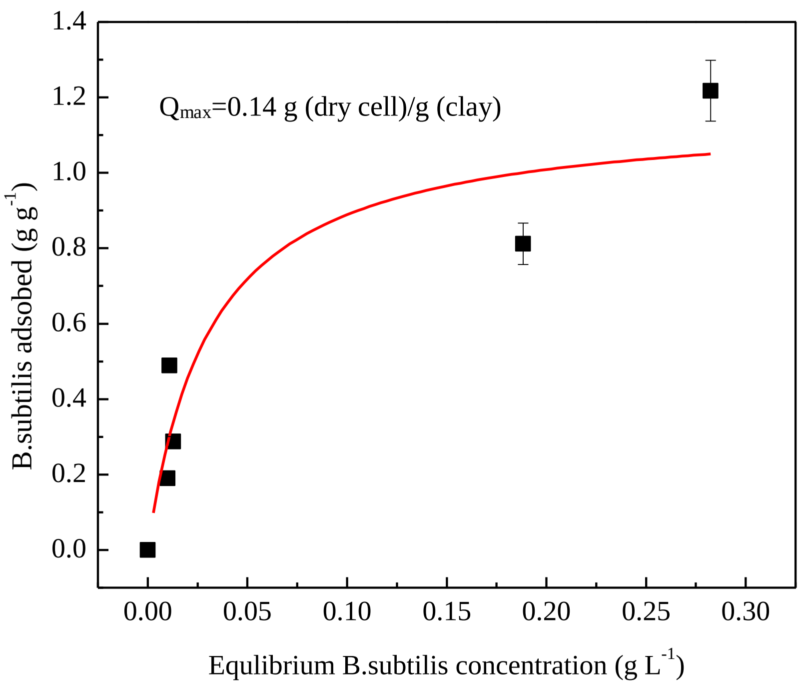

Figure S1. Adsorption of *B. subtilis* (wet) onto montmorillonite at pH 8, 28 ℃, (An inoic strength of 0.01 M was provided by $NaNO_3$, the solid line represents fit curves for Langmuir equations. The ratio of wet to dry weight biomass is 9:1).

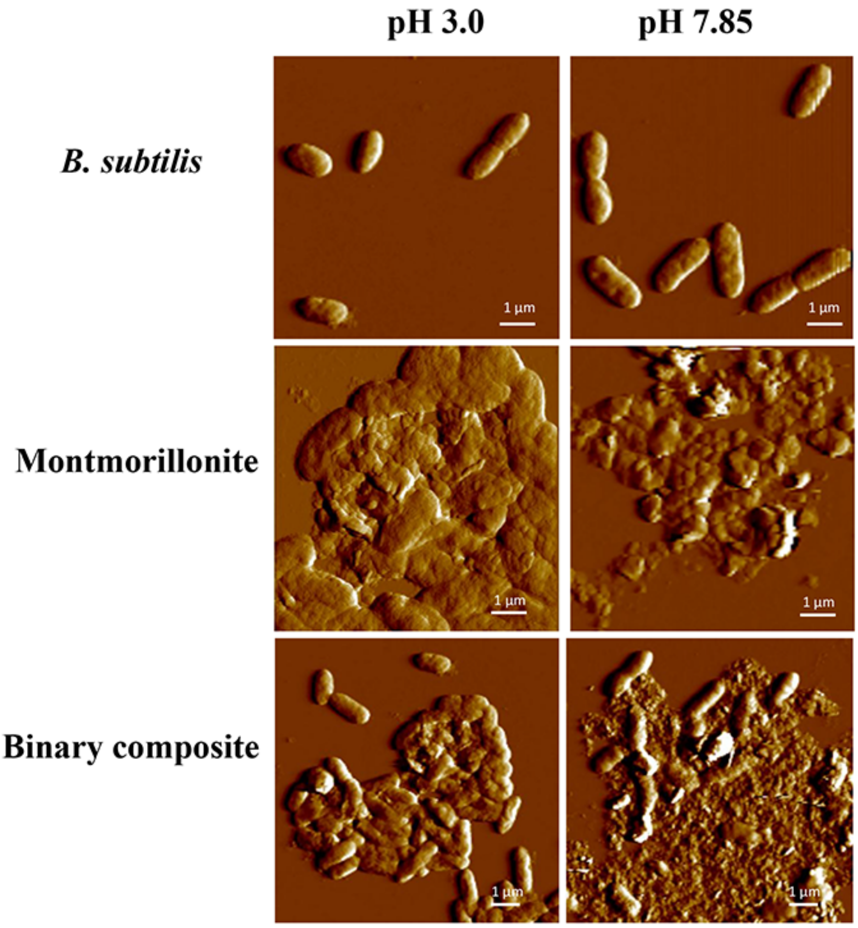

Figure S2. AFM image of *B.subtilis*, montmorillonite and montmorillonite-*B.subtilis* composite at pH 3.0 and pH 7.85. Morphology measurements of the composite was followed the procedure outlined by Huang et al. (2015).

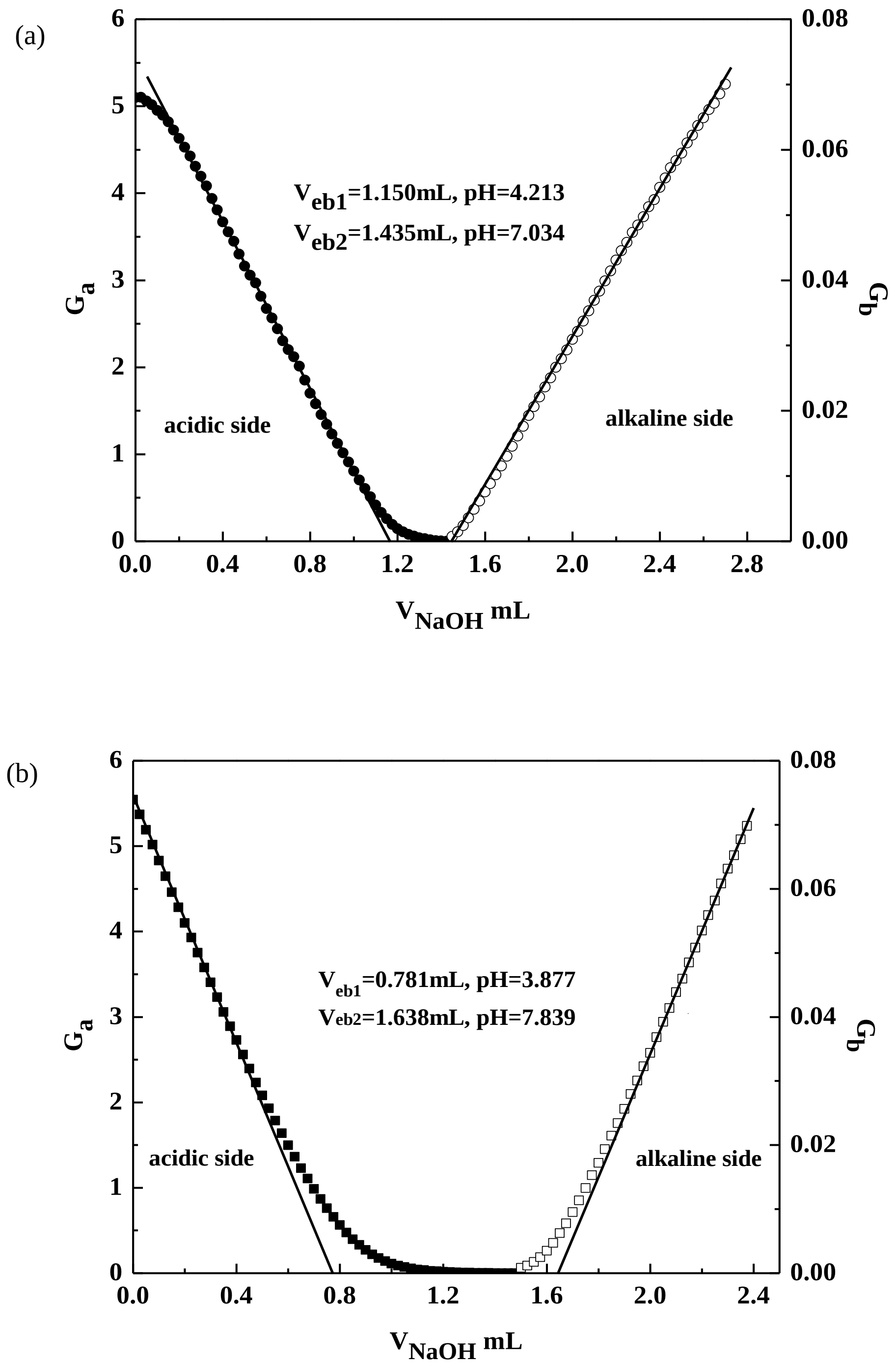

Figure S3. Gran plots of titration systems with 1 g L^{-1} montmorillonite (a) and *B. subtilis* (b) in 0.01 M $NaNO_3$ solution. The open and filled squares denote the titration data for the sample on the acidic side and on the alkaline side, respectively. The solid line represents the tangential line of the titration curve.

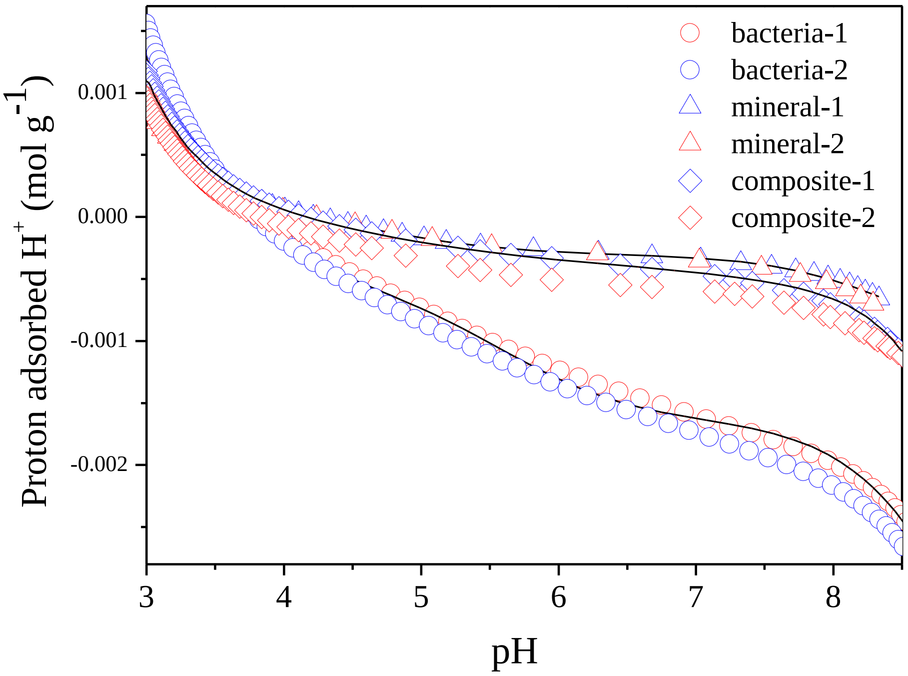

Figure S4. Potentiometric titration data of montmorillonite (a), *B. subtilis* (b) and montmorillonite-*B. subtilis*(c) in 0.01M $NaNO_3$ solution at 25 ℃ (symbols are data points, line are model fits).

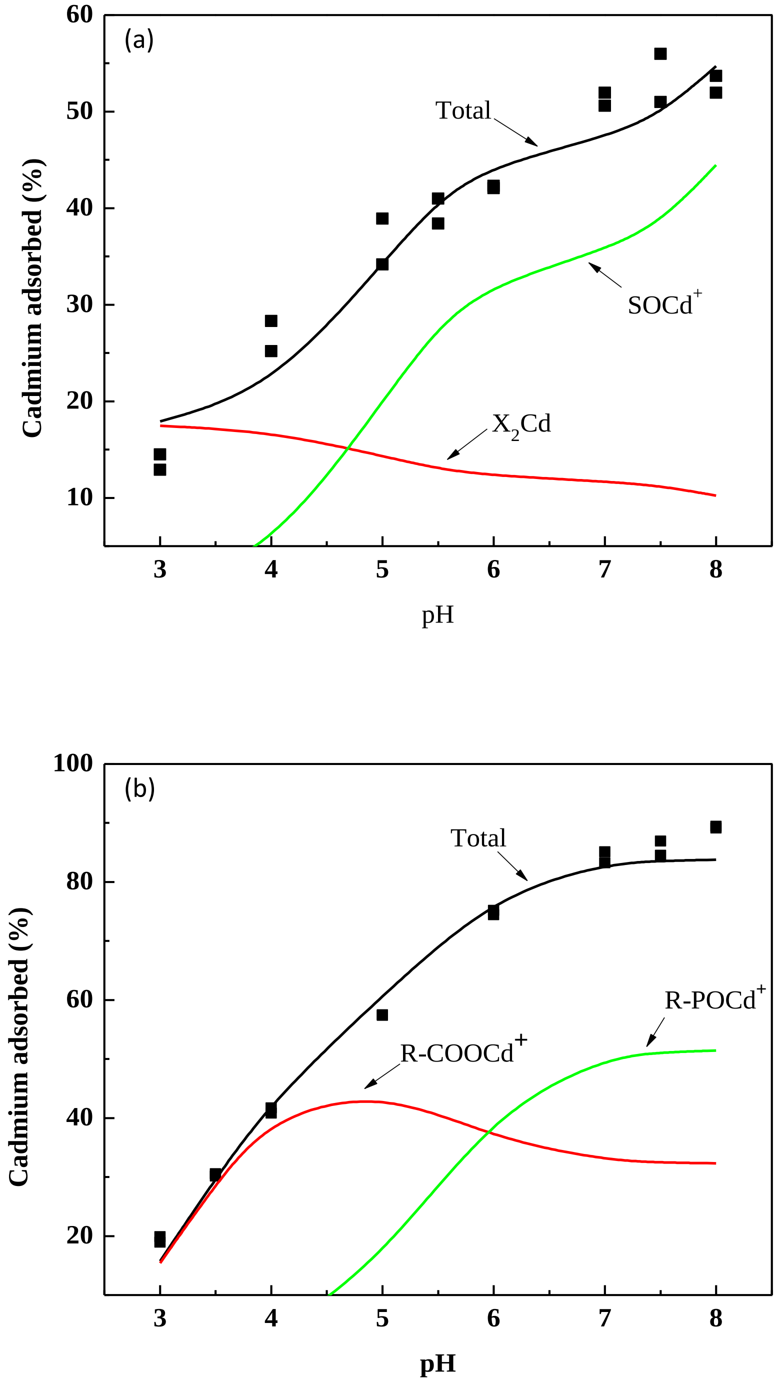

Figure S5. Speciation diagrams for cadmium adsorption onto montmorillonite (a) and *B. subtilis* (b) at 28 ℃, calculated from the surface complexation models (filled squares represent the experimental adsorption data).

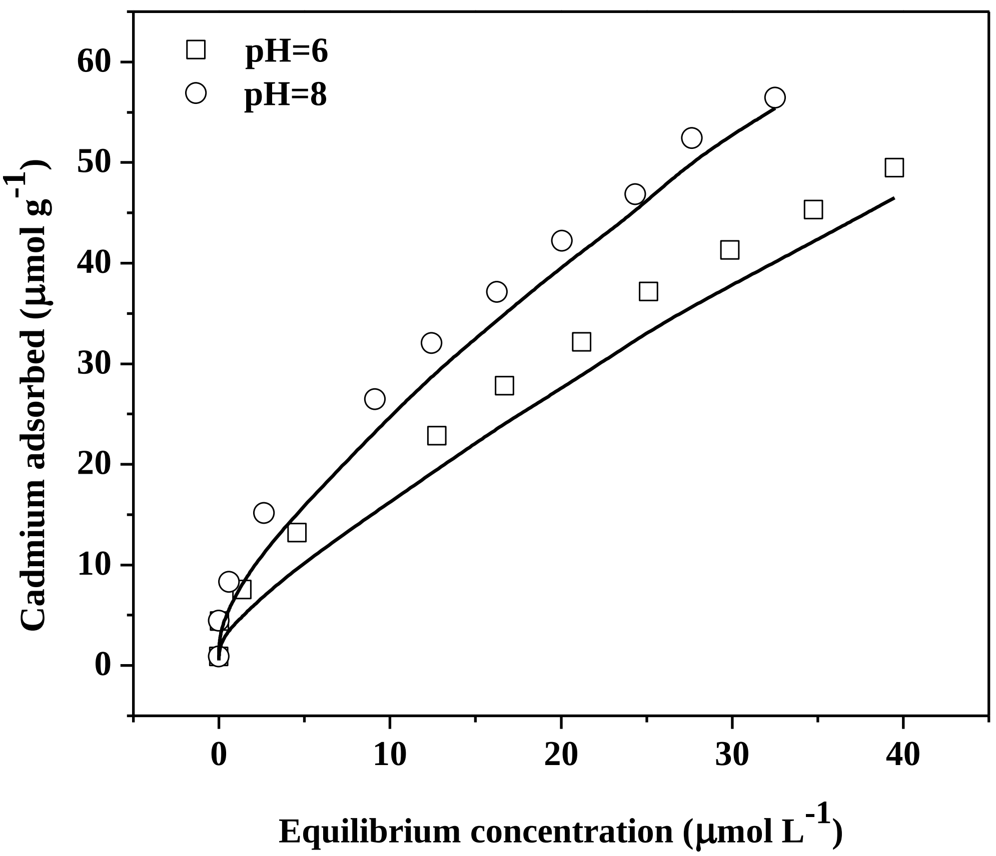

Figure S6. Adsorption isotherms of Cd on montmorillonite–*B. subtilis* composite (1 g L^{-1}) at different pH values in the presence of 0.01 M $NaNO_3$ (symbols are data points and lines are model fits).

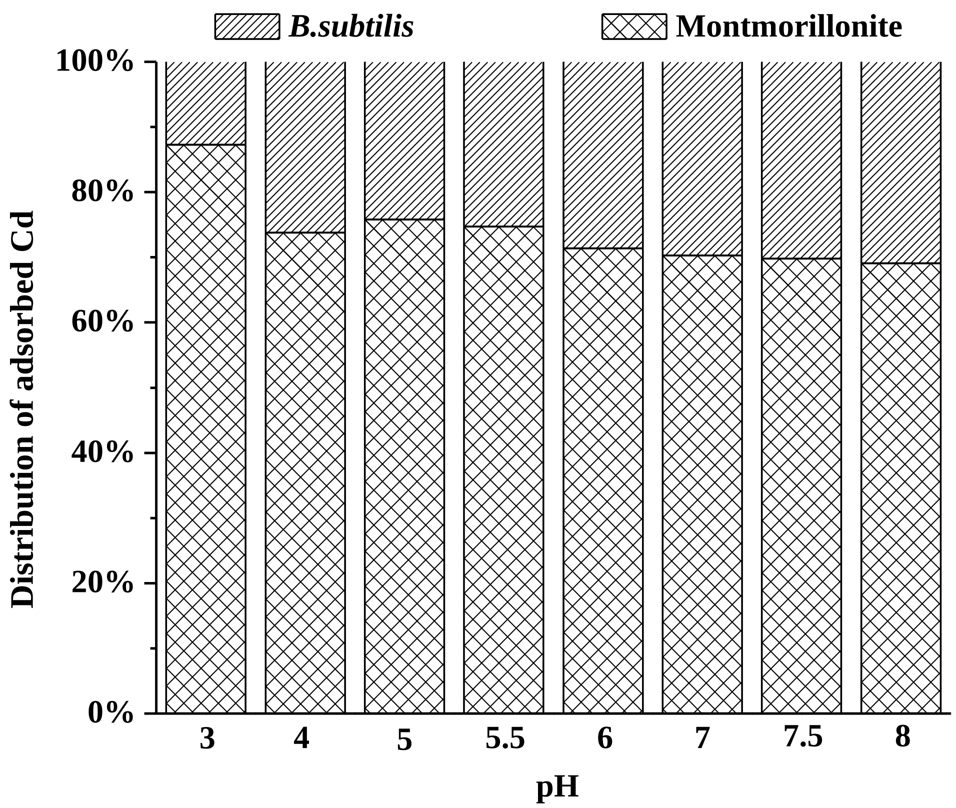

Figure S7. Distribution ratio of total adsorbed Cd between montmorillonite and *B. subtilis* at different pH values in the composite determined from model prediction.

Table S1. Surface complexation model parameters for Cd(II) sorption on montmorillonite.

Surface area (m^2/g)		800[a]
Total concentration of sites (mmol/g)		
SOH		0.30[b]
WOH		1.16[b]
X^-		0.87[a]
Specific capacitance (F/m^2)		4.5[a]
Surface reactions		
$LogK_{XH}$	$X^- + H^+ \Leftrightarrow XH$	-2.2[a]
$LogK_{XNa}$	$X^- + Na^+ \Leftrightarrow XNa$	1.4[a]
$LogK_{SO^-}$	$SOH \Leftrightarrow SO^- + H^+$	-4.83 ±0.06[b]
$LogK_{SOH2^+}$	$SOH + H^+ \Leftrightarrow SOH_2^+$	1.86 ±0.06[b]
$LogK_{WO^-}$	$WOH \Leftrightarrow WO^- + H^+$	-8.36 ±0.08[b]
$LogK_{X2Cd}$	$2X^- + Cd^{2+} \Leftrightarrow X_2Cd$	8.30 ±0.04[b]
$LogK_{SOCd^+}$	$SOH + Cd^{2+} \Leftrightarrow SOCd^+ + H^+$	-1.68 ±0.005[b]

[a] Fixed at those determined for montmorillonite (Tertre et al., 2006 and Soltermann et al., 2014).

[b] Determined from fitting potentiometric titration data.

Table S2. Surface complexation model parameters for Cd(II) sorption on *B. subtilis*.

Surface area (m^2/g)		140
Total concentration of sites (mmol/g)		
R-COOH		0.161 ±0.03[a]
R-POH		0.123 ±0.001[a]
R-OH		1.934 ±0.06[a]
Specific capacitance (F/m^2)		10
Surface reactions		
$\log K_{R\text{-}COO^-}$	$R\text{-}COOH \Leftrightarrow R\text{-}COO^- + H^+$	-3.32 ±0.08[a]
$\log K_{R\text{-}PO^-}$	$R\text{-}POH \Leftrightarrow R\text{-}PO^- + H^+$	-5.38 ±0.02[a]
$\log K_{R\text{-}O^-}$	$R\text{-}OH \Leftrightarrow R\text{-}O^- + H^+$	-9.34 ±0.05[a]
$\log K_{R\text{-}COOCd^+}$	$R\text{-}COO^- + Cd^{2+} \Leftrightarrow R\text{-}COOCd^+$	2.54 ±0.005[a]
$\log K_{R\text{-}POCd^+}$	$R\text{-}PO^- + Cd^{2+} \Leftrightarrow R\text{-}POCd^+$	2.87 ±0.02[a]

[a] Determined from fitting potentiometric titration data.

Reference:

Huang, Q., Wu, H., Cai, P., Fein, J. B., and Chen, W.: Atomic force microscopy measurements of bacterial adhesion and biofilm formation onto clay-sized particles. *Sci. Rep.* 5, 16857, 2015.