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A Universal Synergistic Rule of Cd(II)-Sb(V) Coadsorption to Typical Soil Mineral and Organic Components

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Heavy metals and metalloids are common cooccurrence in contaminated soils, making their behaviors more complex than their individual presences. Adsorption to soil minerals and organic components determines the solubility and mobility of heavy metals. However, little information is available regarding coadsorbing metals (e.g., Cd) and metalloids (e.g., Sb) to soil components, and whether there is a universal coadsorption rule needs to be illuminated. This study investigated the coadsorption behaviors of Cd(II) and Sb(V) to goethite, kaolinite, and bacteria (*Bacillus cereus*) at both acidic (pH 4.5) and alkaline pH (pH 8.5). Equilibrium adsorption experiments, coupled with scanning electron microscopy- (SEM-) energy-dispersive X-ray spectrum (EDS) and X-ray photoelectron spectroscopy (XPS), were applied to determine the batch adsorption phenomena and possible mechanisms. Batch results showed that Cd(II) adsorption was greater at pH 8.5 whereas Sb(V) adsorption was greater at pH 4.5. The presence of Cd or Sb promoted each other's adsorption to goethite, kaolinite, and bacteria, but slight differences were that Sb(V) preferred to enhance Cd(II) adsorption at acidic pH, whereas Cd(II) was more able to increase Sb(V) adsorption at alkaline pH. SEM-EDS analyses further showed that the distribution of Cd and Sb was colocalized. The surface FeOH, AlOH, and COOH groups participated in the binding of Cd(II) and Sb(V), probably through the formation of inner-sphere complexes. Two possible ternary complexes, i.e., sorbent-Cd^{2+}-$Sb(OH)_6^-$ and sorbent-$Sb(OH)_6^-$-Cd^{2+}, were possibly formed. Both the charge effect and the formation of ternary complexes were responsible for the collaborative coadsorbing of Cd-Sb. The universal synergistic rule obtained suggests that current models for predicting Cd(II) or Sb(V) sequestration based on single systems may underestimate their solid-to-liquid distribution ratio in a coexistence situation. The results obtained have important implications for understanding the chemical behavior of Sb and Cd in contaminated soils.

1. Introduction

Soils contaminated with both elevated concentrations of heavy metals (e.g., Cd and Pb) and metalloids (e.g., As and Sb) are common in mining and smelting-impacted regions. For example, Sb/As-Cd combined pollution often occurs in soils surrounding mines due to the concomitant presence of Cd in Sb/As-containing ores [1–4]. The chemical properties of metals and metalloids are distinctly different; i.e., Sb and As commonly exist as oxyanion whereas Cd presents as cation, which makes a big difference in their reactivity, bioavailability, mobility, and fate in the environment. Moreover, the coexistence of metal cations and anions poses a higher risk to biologic organisms and ecological safety than their individual

presences [5]. Unfortunately, studies focusing on the behaviors of coexisting metals-metalloids in soils are rare.

Adsorption-desorption is an important process determining the solubility and partitioning of metal pollutants between the solid and aqueous interfaces. The most important interfaces include phyllosilicates, metal (oxyhydr)oxides, organic matter, and microbes [6–11]. Metal cations and metalloids show quite different affinities towards soil components [12]. For metal cations, favorable adsorption is commonly observed on organic colloids such as humus, microbes, and extracellular secretions at environmentally relevant pH [13–18]. These organic constituents exhibit negative surface charge and abundant functional groups including carboxyl, phosphate, amino, phenolic hydroxyl, and

sulfhydryl [19–22], showing a strong ability to complex metal cations to form stable inner-sphere-type complexes. As for metalloids, they are inclined to bind to metal (oxyhydr)oxides [23–26] rather than the organic constituents. Strong inner-sphere surface complexes and structural incorporation were observed during As and Sb adsorption to Fe/Al/Mn (oxyhydr)oxides [27–34]. Several studies also demonstrated that pH is a dominant influencing factor; i.e., lower pH favors metalloid adsorption whereas higher pH favors metal cation adsorption.

There is an increasing number of studies investigating the coadsorption characteristics of metal-metalloid to soil metal (oxyhydr)oxides. For example, Jiang et al. [30] showed that the adsorption of Cd(II) on goethite was enhanced in the presence of As(V), which could be interpreted by the decreased electrostatic potential with adsorbed AsO_4^{3-} and the formation of a Cd-As-goethite complex. In contrast, Cd(II) did not affect As(V) adsorption quantity but changed its coordination environments such as the As-Fe distance [30]. Carabante et al. [35] discovered that Zn(II) had no effect on As(V) adsorption to ferrihydrite at pH 4 but significantly enhanced adsorption at pH 8, possibly due to the formation of arsenate-zinc hydroxide carbonate complexes. For the Cd(II)-Sb(V) system, Liu et al. [36] observed a positive effect of Cd(II) on Sb(V) adsorption to Fe-Mn binary oxides, owing to the increased ζ-potential and the formation of Cd(II)-Sb(V) precipitates. Similar metal-metalloid-mineral precipitates were also observed such as Cu(II)-As(V)-goethite [37] and Zn(II)-As(V)-goethite [38].

Although coadsorbing metal-metalloids to metal (oxyhydr)oxides have been well documented, information regarding clay mineral systems is rare. Clay minerals, a group of hydrous aluminum silicates, are also an important mineral host for heavy metals/metalloids in soils [6]. Clay minerals have completely different surface charge characteristics compared to metal (oxyhydr)oxides, which might show different impacts on coadsorbing metals-metalloids. In addition to minerals, soil organic constituents such as humus and microbes also play an important role in metal sequestration [39]. There is also an urgent need to investigate the behaviors of coadsorbing metal-metalloids in organo systems.

This investigation was aimed at elucidating whether there is a universal coadsorption rule of Cd-Sb to typical soil mineral and organic components and how this coadsorption behavior affects the mobility and fate of Cd and Sb in contaminated soils. We selected two kinds of minerals, i.e., kaolinite, a typical clay mineral, and goethite, a typical iron oxide, and one representative organic component, i.e., bacteria (*Bacillus cereus*), under both acidic and alkaline pH. Batch adsorption coupled with various spectroscopic tools was applied. The results of this study will provide a new perspective for realizing how Sb(V)-Cd(II) cointeracts with soil components, which helps predict their mobility and fate in contaminated soils and sediments.

2. Materials and Methods

2.1. Materials. Goethite was synthesized following the procedures described in Schwertmann et al. [40], by hydrolyzing a Fe(NO₃)₃ solution to pH 12, and aged at 60°C for 24 h. Kaolinite was purchased from the Clay Minerals Society. The <2 μm clay-sized fractions were separated via a sedimentation procedure reported in Rong et al. [41]. The *Bacillus cereus* is an autochthonous Gram-positive soil bacterium (GenBank accession number is MH34583). Bacterial cells were cultured in a Luria-Bertani nutrient medium at 28°C. The biomass was obtained by centrifugation, and the cells were suspended in the electrolyte (0.1 M KNO₃) to form a parent solution and stored at 4°C before use.

2.2. Batch Experiments. Adsorption experiments were conducted in a batch process at room temperature (25°C). Sb(V) and Cd(II) stock solutions were prepared from KSb(OH)₆ and Cd(NO₃)₃, respectively. Adsorption samples, containing 0.05 g/L sorbent (goethite/kaolinite/*Bacillus cereus*) and 0.2 mM adsorbate (Cd and/or Sb), were prepared in a 0.1 M KNO₃ electrolyte. Three different systems were considered: single Cd, single Sb, and binary Cd-Sb (1 : 1 molar ratio). The pH of the adsorption suspension was adjusted to either pH 4.5 or 8.5 using dilute NaOH or HNO₃, and the suspension was placed on an end-over-end shaker for 24 h. Adsorption suspensions were then centrifuged at 4500 g. The supernatants were filtered through a 0.45 μm syringe filter, acidified with 1% HNO₃, and analyzed using Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES). The residual thick pastes left in the adsorption experiments were freeze-dried for SEM-EDS and XPS analyses. All batch experiments were conducted in triplicate.

2.3. Characterization. Scanning electron microscopy was recorded on a field emission scanning electron microscope (FE-SEM, Quanta 250, USA), equipped with a Flat QUAD probe (Bruker Quantax) for energy-dispersive spectroscopy (EDS) analysis. The ζ-potentials of goethite, kaolinite, and *Bacillus cereus* cell were determined using a ζ-potential analyzer (Zetaplus90, Brookhaven). X-ray photoelectron spectroscopy (XPS) was recorded using an X-ray photoelectron spectrometer (Thermo Fisher Scientific, USA) with a KRATOS Axis Ultra X-ray source (1486.7 eV). An energy range of 0–1100 eV was used with a step size of 1 eV for a wide-scan spectrum, and the high-resolution scans were recorded with a step size of 0.05 eV. The C 1s peak at 284.8 eV was used as an internal standard calibration peak for charge correction. The Shirley background and Gaussian/Lorentzian were set up to 20%.

3. Results and Discussion

3.1. Synergistic Coadsorption of Cd(II)-Sb(V) to Goethite, Kaolinite, and Bacteria. In goethite systems, Sb(V) adsorption was larger at pH 4.5 than at pH 8.5, with an equilibrium Sb(V) adsorption of 1.42 and 1.17 mmol/g, respectively (Table 1, batches 1 and 4). The uptake of Cd(II) was greater at pH 8.5 than at pH 4.5, with the final Cd adsorption of ~1.64 and 0.4 mmol/g, respectively (Table 1, batches 5 and 2). Our findings agree with previous observations [14, 34]. Goethite normally has a pH$_{pzc}$ (zero point of charge) around

TABLE 1: Summary of experimental conditions and final adsorption of Sb(V) and Cd(II) for the batch experiments.

	Batch experiment	Initial concentration (mmol/L)		pH	Adsorption (mmol/g)	
		Sb(V)	Cd(II)		Sb(V)	Cd(II)
Goethite	1	0.2			1.42 ± 0.04	
	2		0.2	4.5		0.40 ± 0.01
	3	0.2	0.2		1.60 ± 0.03	0.70 ± 0.07
	4	0.2			1.17 ± 0.01	
	5		0.2	8.5		1.64 ± 0.02
	6	0.2	0.2		2.58 ± 0.14	1.99 ± 0.02
Kaolinite	7	0.2			1.14 ± 0.03	
	8		0.2	4.5		0.29 ± 0.01
	9	0.2	0.2		1.50 ± 0.02	1.17 ± 0.01
	10	0.2			0.64 ± 0.01	
	11		0.2	8.5		1.23 ± 0.06
	12	0.2	0.2		1.74 ± 0.01	1.99 ± 0.01
Bacteria	13	0.2			0.28 ± 0.01	
	14		0.2	4.5		1.03 ± 0.01
	15	0.2	0.2		0.59 ± 0.03	1.63 ± 0.03
	16	0.2			0.20 ± 0.01	
	17		0.2	8.5		2.33 ± 0.01
	18	0.2	0.2		1.05 ± 0.01	2.67 ± 0.07

7.5 [42]. At pH 4.5, goethite is positively charged (ζ-potential = 17.33 mV, Table 2); an electrostatic attraction between Sb(V) oxyanions and goethite could facilitate adsorption, whereas a strong electrostatic repulsion between Cd(II) and the surface would inhibit adsorption. The opposite is true at pH 8.5. In binary systems, both Sb(V) and Cd adsorptions were greater than those in single systems. Specifically speaking, Sb(V) removal increased to 1.60 and 2.28 mmol/g, respectively, at pH 4.5 and 8.5 (Table 1, batches 3 and 6); Cd adsorption raised to 0.70 and 1.99 accordingly. It is therefore concluded that Cd-Sb coadsorption on goethite is a synergistic process. Notably, the increment in Sb(V) adsorption was much greater (~120%) at pH 8.5 than at pH 4.5 (~13%), whereas the enhancement in Cd(II) removal was greater (~75%) at pH 4.5 than at pH 8.5 (~21%).

In kaolinite systems, the removal of Sb(V) was greater at pH 4.5 than at pH 8.5 (Table 1, batches 7 and 10); the opposite was true for Cd(II) (Table 1, batches 8 and 11). This adsorption trend with pH is similar to that in goethite systems and agrees with previous observations in literature [43, 44]. Kaolinite is negatively charged at both pH 4.5 and 8.5 (Table 2); the increased negative charge with increasing pH may explain the different adsorption properties for Sb(V) and Cd(II). In binary systems, Sb(V) adsorption was increased to 1.50 and 1.75 mmol/g, respectively, at pH 4.5 and 8.5 (Table 1, batches 9 and 12), corresponding to an increment of ~32% and 173%, respectively. The uptake of Cd(II) was increased by ~315% and 62%, respectively, at

TABLE 2: The zeta potentials (mV) of goethite, kaolinite, and bacteria at different pH.

	pH	Zeta potential (mV)
Goethite	4.5	17.33
	8.5	-23.73
Kaolinite	4.5	-6.12
	8.5	-25.01
Bacteria	4.5	-16.68
	8.5	-56.79

pH 4.5 and 8.5. The presence of Cd(II) was more able to promote Sb(V) adsorption at alkaline pH, while Sb(V) was more capable of facilitating Cd(II) adsorption at acidic pH, which is consistent with the trend in goethite systems.

In bacteria systems, the uptake of Sb(V) was larger at pH 4.5 than at pH 8.5, with a final Sb(V) adsorption of 0.28 and 0.20 mmol/g, respectively (Table 1, batches 13 and 16). The much lower Sb(V) adsorption on bacteria than those on goethite and kaolinite is mainly because of the stronger repulsion between Sb(V) oxyanions and more negatively charged bacterial cells (see ζ-potentials in Table 2). The adsorption of Cd(II) was much larger at pH 8.5 than at pH 4.5 (Table 1, batches 14 and 17). In binary systems, Sb(V) uptake was increased by ~111% and 425%, respectively, at pH 4.5 and 8.5, compared to those in single systems. The adsorption of Cd had increased by ~58% and 15%, respectively, at pH 4.5 and 8.5. Similar to goethite and

(a)   (b)   (c)
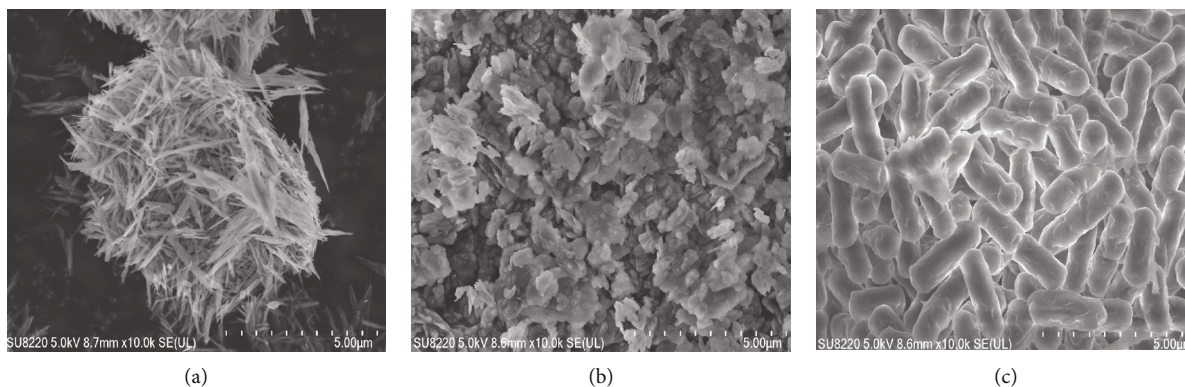
FIGURE 1: SEM images of (a) goethite, (b) kaolinite, and (c) *Bacillus cereus* cell.
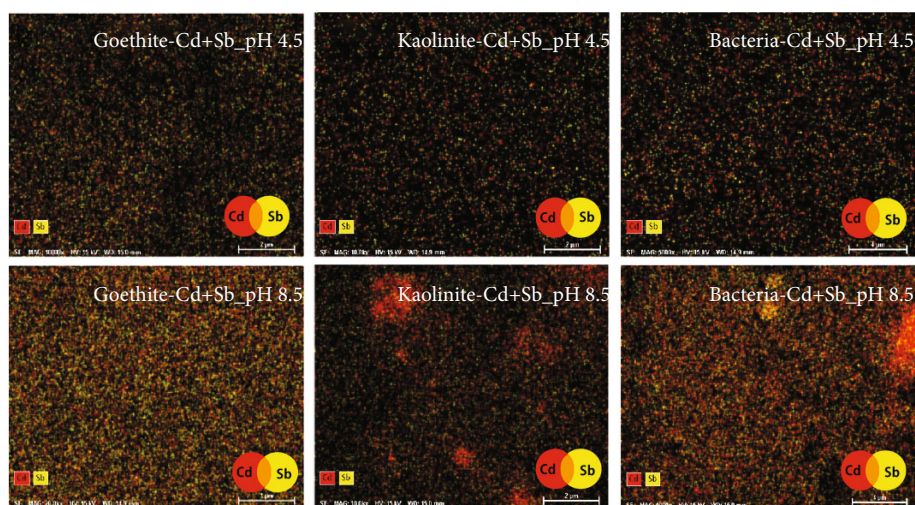

FIGURE 2: SEM-ED mapping of goethite, kaolinite, and *Bacillus cereus* cell after the sorption of Cd(II) and Sb(V) at pH 4.5 and 8.5.
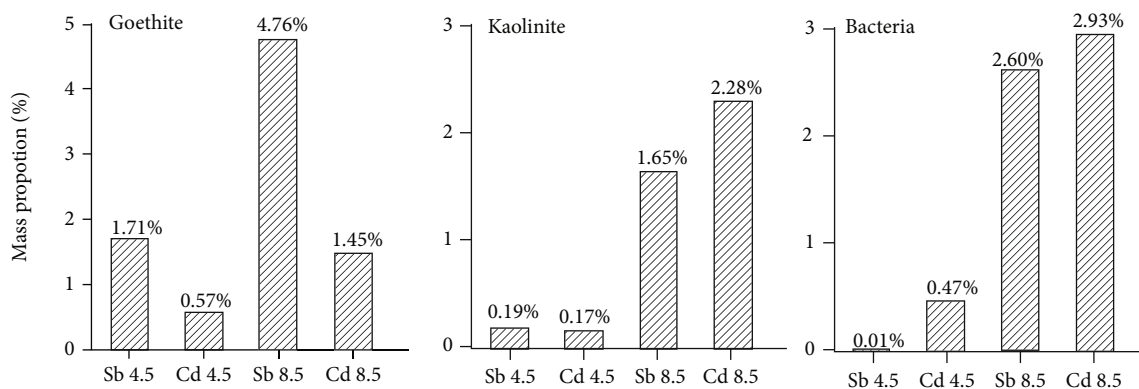

FIGURE 3: Mass percentage of Cd(II) and Sb(V) in goethite, kaolinite, and *Bacillus cereus* cell. Data are produced from Figure 2.

kaolinite systems, the promotion in Sb(V) adsorption was more pronounced at higher pH, whereas lower pH was more favorable to promote Cd(II) adsorption.

Overall, the batch results demonstrate a synergistic coadsorption behavior of Cd(II)-Sb(V) to typical soil clay minerals, iron (oxyhydr)oxides, and bacteria. The presence of Sb(V) significantly enhances Cd(II) adsorption at acidic

pH, whereas Cd(II) prominently facilitates Sb(V) adsorption at alkaline pH.

3.2. SEM-EDS Analyses. Typical morphology pictures of goethite, kaolinite, and *Bacillus cereus* are shown in Figure 1. The synthesized goethite comprises <2 μm needle-type crystal. Kaolinite shows a layered hexagonal shape with a size
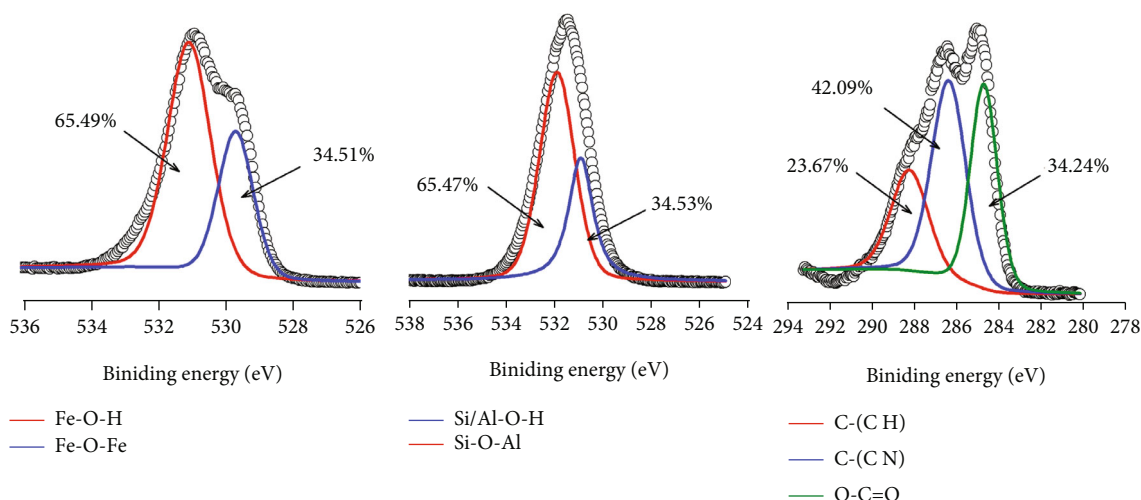
FIGURE 4: High-resolution O 1s XPS spectra of goethite and kaolinite and C 1s XPS spectrum of the *Bacillus cereus* cell.
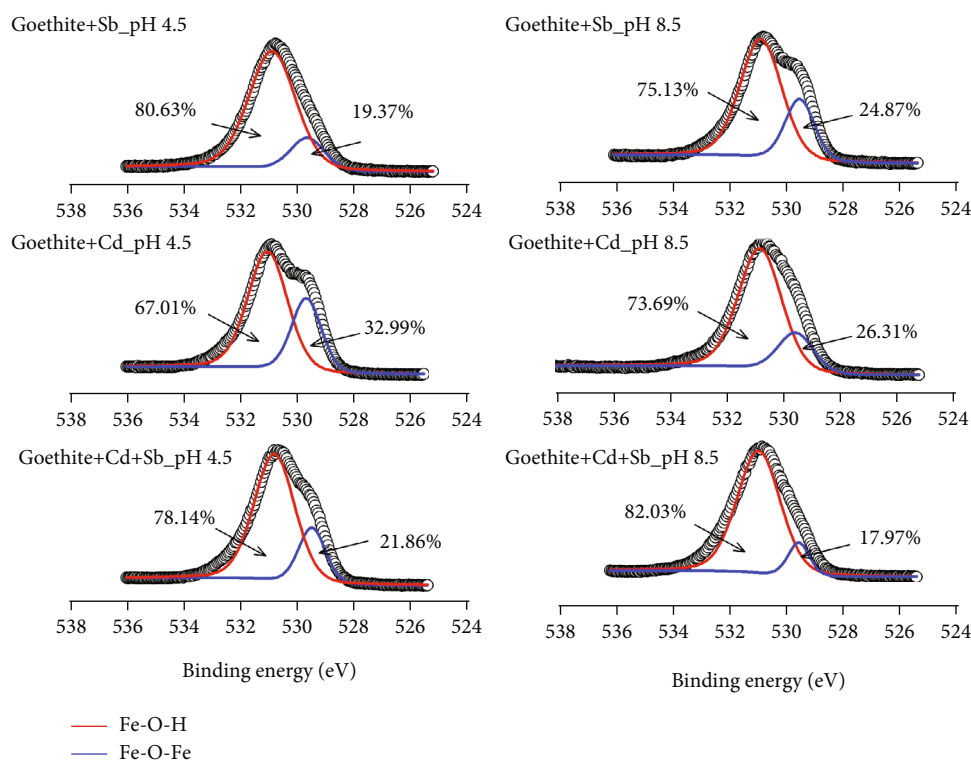

FIGURE 5: High-resolution O 1s XPS spectra of goethite after the sorption of Cd(II) and/or Sb(V).

mostly smaller than $2\,\mu m$. *Bacillus cereus* cells yield a rod shape with cell length and width of $\sim 3.0\,\mu m$ and $1\,\mu m$, respectively.

Two-color SEM-EDS elemental maps of the distribution of Sb (yellow) and Cd (red) in goethite, kaolinite, and *Bacillus cereus* are shown in Figure 2. There are few separated red or yellow areas (mostly orange, red+yellow), indicating that the distribution of Sb and Cd is positively correlated. This could be due to the formation of the ternary sorbent-Sb-Cd complexes at the same coordinated sites. The elemental mass percentage results (Figure 3) show clearly that kaolin-ite, goethite, and bacteria adsorb much more Cd/Sb at pH 8.5 than at pH 4.5 in the coexisting situation. This may indicate that Cd(II) and Sb(V) could be more easily coad-sorbed by soil components in an alkaline environment.

3.3. XPS Analyses. To reveal the underlying mechanisms, goethite, kaolinite, and *Bacillus cereus* before and after the binding of Cd and/or Sb were characterized by XPS (Figures 4–7). XPS is a powerful tool for surface functional group analyses. For goethite, the O 1s spectrum can be sub-divided into Fe–O–Fe (529.67 eV) and Fe–O–H (531.04 eV)
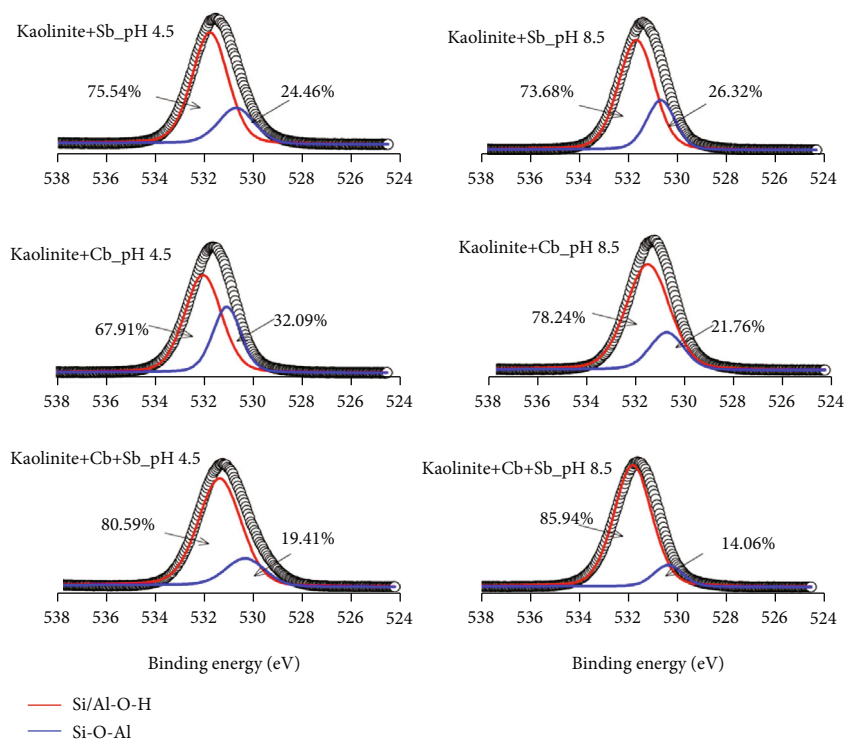
Kaolinite+Sb_pH 4.5

75.54%   24.46%

538 536 534 532 530 528 526 524

Kaolinite+Sb_pH 8.5

73.68%   26.32%

538 536 534 532 530 528 526 524

Kaolinite+Cb_pH 4.5

67.91%   32.09%

538 536 534 532 530 528 526 524

Kaolinite+Cb_pH 8.5

78.24%   21.76%

538 536 534 532 530 528 526 524

Kaolinite+Cb+Sb_pH 4.5

80.59%   19.41%

538 536 534 532 530 528 526 524

Kaolinite+Cb+Sb_pH 8.5

85.94%   14.06%

538 536 534 532 530 528 526 524

Binding energy (eV)   Binding energy (eV)

— Si/Al-O-H
— Si-O-Al

FIGURE 6: High-resolution O 1s XPS spectra of kaolinite after the sorption of Cd(II) and/or Sb(V).

Bacteria+Sb_pH 4.5

51.64%

28.09%   20.27%

294 292 290 288 286 284 282 280 278

Bacteria+Sb_pH 8.5

42.20%

26.27%   31.38%

294 292 290 288 286 284 282 280 278

Bacteria+Cd_pH 4.5

38.43%

29.42%   32.15%

294 292 290 288 286 284 282 280 278

Bacteria+Cd_pH 8.5

46.68%

31.37%   21.95%

294 292 290 288 286 284 282 280 278

Bacteria+Cd+Sb_pH 4.5

45.02%

32.62%   22.36%

294 292 290 288 286 284 282 280 278

Bacteria+Cd+Sb_pH 8.5

42.03%

34.61%   23.36%

294 292 290 288 286 284 282 280 278
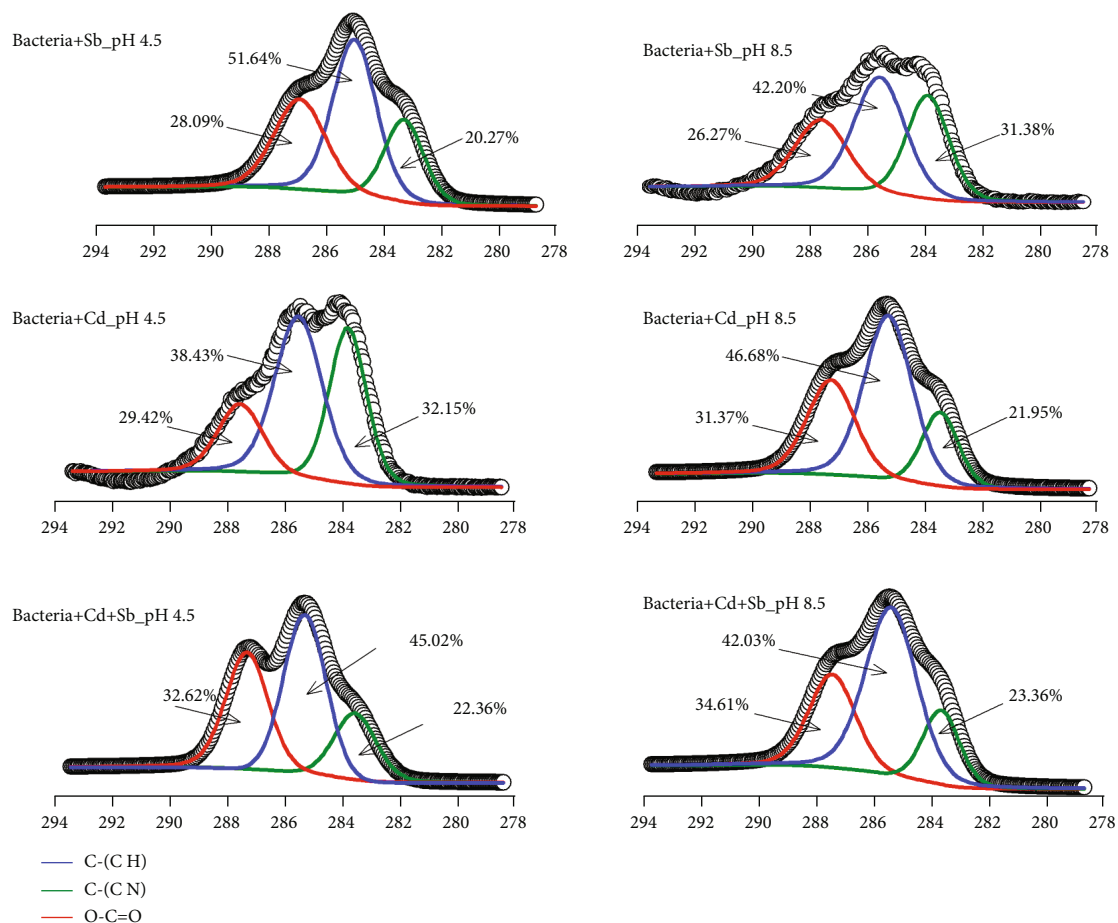
— C-(C H)
— C-(C N)
— O-C=O

FIGURE 7: High-resolution C 1s XPS spectra of the *Bacillus cereus* cell after the sorption of Cd(II) and/or Sb(V).
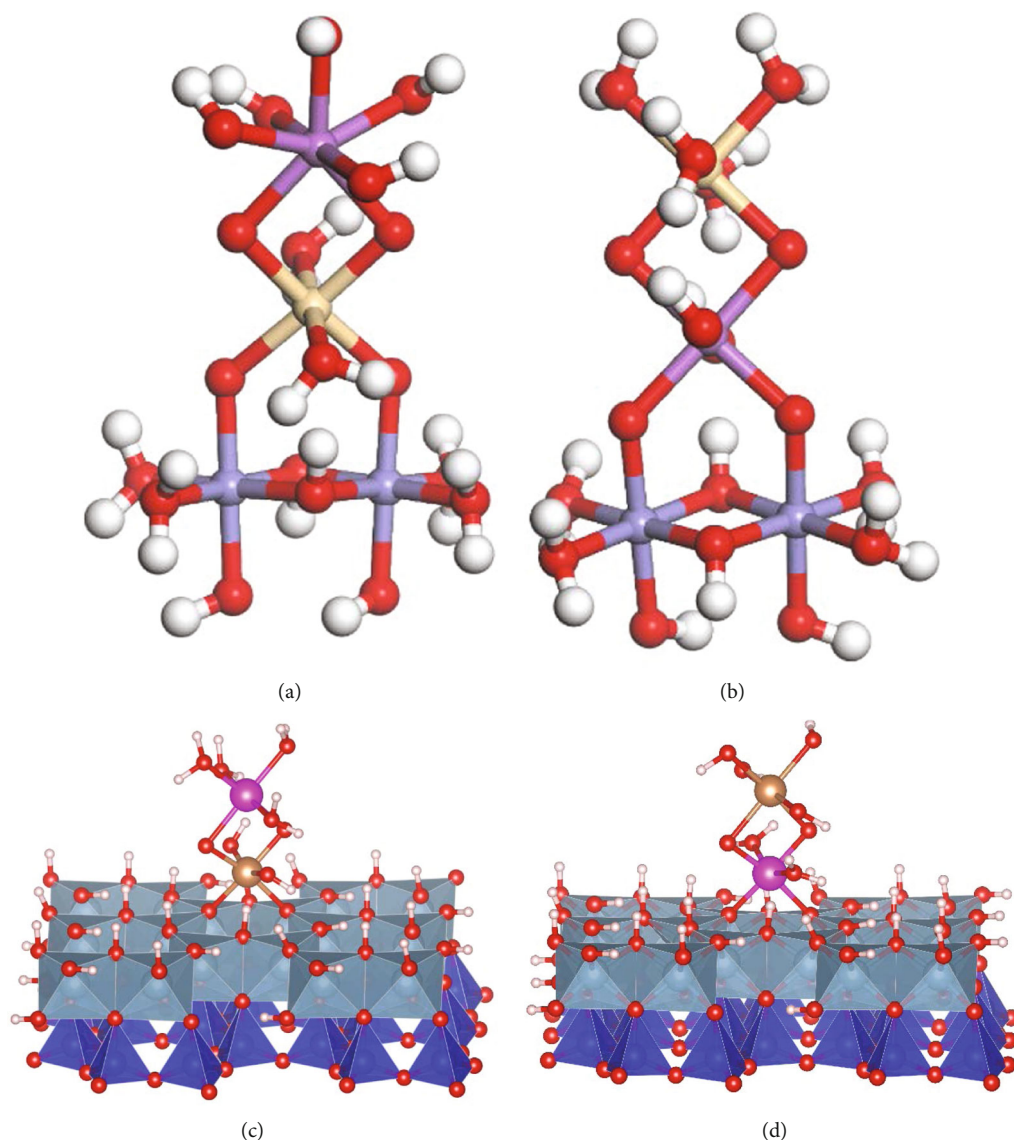
(a) (b)

(c) (d)

FIGURE 8: The structures of two possible ternary complexes on (a, b) goethite and (c, d) kaolinite.

[45]. The peak intensity of Fe-O-H is much higher (65.49%) than that of Fe–O–Fe (34.51%) (Figure 4), indicating the presence of abundant hydroxyl functional groups on the surface. For kaolinite, the O 1s spectrum can be subdivided into O atoms of silanol (≡SiOH) and aluminol (≡AlOH) on the basal/edge surface and O atoms bridging Si and Al (Si–O–Al) [44]. The Si/Al–O–H is located at ~531.91 eV while the Si–O–Al is located at ~530.94 eV, and the proportions are 65.47% and 34.53%, respectively (Figure 4). For bacteria, the peak of C 1s can be decomposed into three peaks which are assigned to the C–C/C–H (284.1 eV), C–O/N (286.5 eV), and O–C=O (288.2 eV), respectively [46].

When Sb(V) and/or Cd(II) adsorb on goethite, there is a significant increase in the Fe–O–H fraction (Figure 5). Specifically, the proportion of Fe–O–H is increased to 80.63%, 67.01%, and 78.14%, respectively, after Sb(V), Cd(II), and Sb(V)-Cd(II) adsorption at pH 4.5 and 75.13%, 73.69%, and 82.03%, respectively, at pH 8.5. These observations demonstrate that the ferric hydroxyl groups of goethite partici-

pate in the binding of Sb(V) and/or Cd(II), possibly through the formation of inner-sphere complexes, i.e., Fe–O–Cd/Sb [34, 47, 48]. These newly formed species would contribute to the increased peak intensity of the surface Fe–O–H. It is also interesting that the changes of Sb(V)-loaded spectra are more evident at pH 4.5, whereas the changes of Cd(II)-loaded spectra are more pronounced at pH 8.5. This again agrees with the batch results that Sb(V) adsorption increases with decreasing pH whereas Cd(II) sorption increases with elevated pH.

When Sb(V) and/or Cd(II) adsorb on kaolinite, the component of Si/Al–O–H is increased to 75.54%, 67.91%, and 80.59%, respectively, after Sb(V), Cd(II), and Sb(V)-Cd(II) adsorption at pH 4.5 (Figure 6). At pH 8.5, the component of Si/Al–O–H is enhanced to 73.68%, 78.24%, and 85.94%, respectively. Therefore, the Si/Al–O–H groups participate in the binding of Cd(II) and/or Sb(V) on kaolinite [49]. The gibbsite basal planes of kaolinite can have variable charges [50], which can complex Cd(II) and Sb(V) to form

various inner-sphere complexes. However, it cannot rule out the presence of outer-sphere complexes from XPS, and a previous study showed that Cd(II) can adsorb both as an outer-sphere complex at the negatively charged basal sites and as an inner-sphere complex at the edges of the clay [44, 51].

When Sb(V) and/or Cd(II) adsorb to bacteria, the component of the O–C=O fraction is increased to 28.09–32.62% at pH 4.5 and 26.42–34.61% at pH 8.5 (Figure 7). The O–C=O fraction is commonly assigned to the carbonyls, carboxylate, and/or aldehydes [52], which make up the peptidoglycan, phospholipid bilayer, lipopolysaccharides, and protein of the cell walls. The increase in this component suggests that carboxylic groups are responsible for the binding of Sb and/or Cd(II) on bacterial surfaces.

It is worth noting that for all sorbents (goethite, kaolinite, and bacteria), the changes of the Fe/Si/Al–O–H and O–C=O components are more evident in binary Sb-Cd systems than in single systems. On the one hand, this may be due to the higher adsorption of Cd-Sb in binary systems. On the other hand, the formation of a ternary sorbent-Cd-Sb or sorbent-Cd-Sb complexes may play a role.

3.4. Possible Mechanisms and Implications. Goethite, kaolinite, and *Bacillus cereus*, represented by the most ubiquitous soil components, play a crucial role in the sequestration of both metals and metalloids. Our results show that Cd(II)-Sb(V) coadsorption is a synergistic process that their sorption in binary systems is larger than that in single systems. Two possible explanations are as follows: (1) one is the charge effect. Because Cd(II) is positively charged whereas Sb(V) is negatively charged, therefore the adsorption of Cd(II) on the surface will facilitate the electrostatic attraction between Sb(V) and the surface and vice versa. (2) The second is the formation of the ternary complexes. As for the studied systems, two types of ternary complexes are possibly formed, one where the adsorbed Cd is near the surface (type A, sorbent-Cd^{2+}-$Sb(OH)_6^-$) and the other where the adsorbed Sb is near the surface (type B, sorbent-$Sb(OH)_6^-$-Cd^{2+}). For example, the structure of type A complexes on the goethite and kaolinite surface is shown in Figures 8(a) and 8(c), while that for type B is shown in Figures 8(b) and 8(d). The fact that Cd(II) and Sb(V) play a promoting role in each other's adsorption onto soil clay minerals and organic constituents is a nice addition to previous findings only concerning Fe (oxyhydr)oxide systems. Collectively, our results combined with previous findings demonstrate a universal synergistic effect regarding the coadsorbing Cd-Sb to soil components. In this scenario, current thermodynamic models for predicting Cd(II) or Sb(V) behaviors based on single-solute systems may underestimate their binding to soil solid phases in a coexistence situation. Our results also show that the promotion effects are dependent on pH; i.e., Sb(V) enhances Cd(II) adsorption more pronouncedly at acidic pH, whereas Cd(II) prominently facilities Sb(V) adsorption at alkaline pH. This reminds us that soil pH must be taken into consideration when evaluating the coadsorption behaviors of Cd-Sb. As soil components commonly interact with each other, it is therefore important to consider mineral-organo interaction when studying Cd-Sb coadsorbing behaviors in the future.

4. Conclusions

This study provides the first systematic evidence for coadsorbing Cd(II)-Sb(V) to typical mineral and organic components. The results show that Cd(II) and Sb(V) adsorption to goethite, kaolinite, and bacterial cells is greater in binary Cd-Sb systems than in their individual presences at both acidic and alkaline pH. Sb(V) is more able to enhance Cd(II) adsorption at acidic pH, whereas Cd(II) is more capable of increasing Sb(V) adsorption at alkaline pH. The distribution of Sb and Cd is colocalized. The ferric hydroxy groups (FeOH) of goethite, the aluminol (AlOH) of kaolinite, and the carboxyl groups of bacteria are responsible for the binding of Cd(II) and Sb(V), via the formation of inner-sphere-type complexes. Two possible ternary complexes are formed when coadsorption occurs, one where Cd is near the surface and the other where Sb is near the surface. All our observations have important implications for predicting Sb and Cd mobility and fate in contaminated soils.

Data Availability

All data, models, and code generated or used during the study appear in the submitted article.

Conflicts of Interest

The authors declare no conflicts of interest.

Authors' Contributions

Min Zhou and Ruijia Yang contributed equally to this work.

Acknowledgments

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