

Article

Study on Floatation Separation of Molybdenite and Talc Based on Crystal Surface Anisotropy

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Abstract: Talcose molybdenite resources are abundant but resource utilization is low. The floatation separation of molybdenite (MoS₂) and talc is challenging due to their similar natural hydrophobicity and layered structures. This study investigates the surface properties and interaction mechanisms between these minerals to improve their separation efficiency. Density functional theory (DFT) calculations confirm that the basal planes of both minerals are hydrophobic, while their edge surfaces are hydrophilic. Atomic force microscopy (AFM) and DLVO theory reveal that molybdenite and talc particles aggregate in neutral/acidic conditions but disperse in alkaline solutions due to altered surface forces. Floatation experiments demonstrate that pulp pH is the key controlling factor—alkaline conditions (pH > 10) effectively reduce hetero-aggregation, enabling selective molybdenite recovery. These findings provide critical insights into optimizing floatation processes for talcose molybdenite ores, enhancing resource utilization.

Keywords: floatation separation; anisotropy; molybdenite; talc; adsorption; DLVO



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1. Introduction

Molybdenum is a very important rare mineral resource that exists largely in oxidized ores and sulfide ores in nature [1]. Due to its excellent characteristics, it is widely used in the metallurgy, machinery, chemical, and aerospace industries, among many other areas [2]. It has become an indispensable metal in modern industry. About 99% of metallic molybdenum comes from molybdenite [3].

Molybdenite (MoS₂), a layered sulfide mineral with a hexagonal crystal structure, exhibits anisotropic surface properties due to its unique S-Mo-S sandwich configuration (Figure 1a). When fractured, two distinct surface types form [4,5]: (1) basal planes resulting from van der Waals force separation between layers [6–8] and (2) edge surfaces created by covalent bond rupture at layer terminations [9,10]. This structural anisotropy leads to significantly different surface characteristics—the basal planes demonstrate superior hydrophobicity and stability compared to the hydrophilic edge surfaces [11–13].

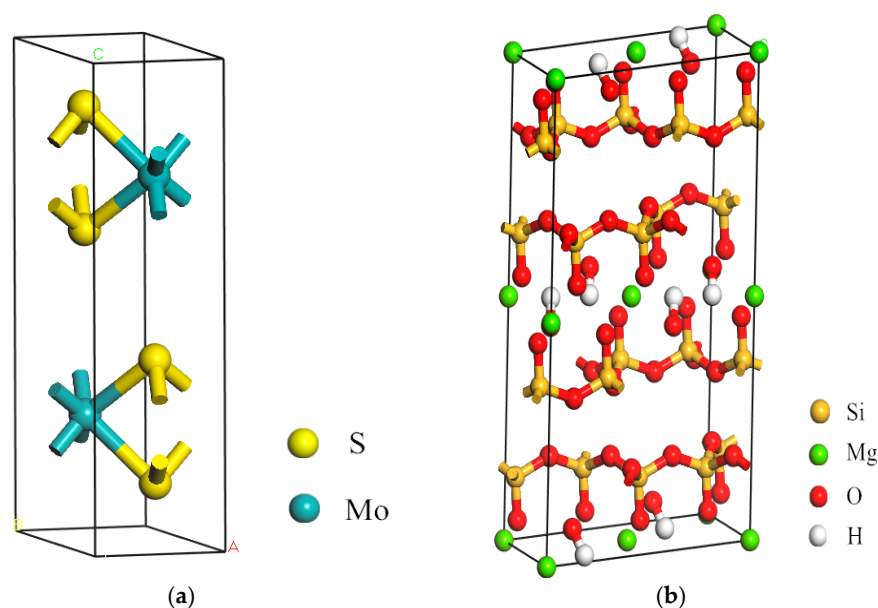


Figure 1. Computed cell models of molybdenite (a) and talc (b).

Talc, a T-O-T-type phyllosilicate (Figure 1b), displays similar structural anisotropy. Its layered structure consists of tetrahedral (T) and octahedral (O) sheets, where T sheets form hexagonal networks of silicon–oxygen tetrahedra and O sheets contain magnesium in an octahedral coordination [14]. Fracture generates two surface types: (1) non-polar, hydrophobic basal planes formed by van der Waals separation and (2) polar, hydrophilic edge surfaces with exposed Si-O and Mg-O bonds that create charged sites [14].

Talc and molybdenite are naturally hydrophobic, so they both have high floatability and their surface properties are similar, which lead to difficulties in separation when talc is present in ores. To fundamentally understand the floatation behavior of molybdenite and talc, it is necessary to study the surface properties of minerals under various conditions. During the past decades, many efforts have been devoted to understanding the surface properties of molybdenite and talc in relation to their mineral processing. Kelebek [15] and others [16–18] studied the wettability and hydrophobicity of molybdenite and talc, pointing out that molybdenite and talc were similar in their structures and properties, and both were hydrophobic minerals. The floatability of talc was even better than that of molybdenite. Therefore, it is key to separate and remove talc from molybdenite effectively. However, due to their small sizes and distinct anisotropic surface characteristics, some of the crucial surface properties of molybdenite and talc, especially in terms of specific faces, remain unclear. In this study, the adsorption energies of H₂O molecules on different crystal faces of minerals are studied through density functional theory. In addition, the surface potentials and interaction forces of different surfaces of molybdenite and talc were investigated by direct surface force measurements with an atomic force microscope (AFM) and classical DLVO (Derjaguin–Landau–Verwey–Overbeek) theory. The results will reveal why talc interferes with the floatation of molybdenite and can provide a theoretical basis for the floatation separation of molybdenite and talc. While the crystal structures of molybdenite and talc are well-documented, their face-specific surface properties and interparticle forces—key to floatation separation—remain poorly understood. This work addresses this gap by integrating DFT, AFM, and DLVO theory to decode the pH-dependent interaction mechanisms, ultimately proposing a practical solution for selective molybdenite recovery.

2. Materials and Methods

2.1. Materials

The raw materials are molybdenite minerals taken from the Luoyang area and talc minerals taken from the Haicheng area in China. They are produced by cleaning, drying, and crushing after manual selection [19]. The raw ore is crushed into small pieces in the first step and sorted by hand and a shaking table to select higher-grade ores. Then, they are ground with a porcelain mill and finally screened to -0.100 mm as the sample with a standard sieve. We use ICP, AAS, XRF, and chem-titrimetry for the chemical multi-element analysis of samples. The test results show that the single-mineral purities of molybdenite and talc are above 95%. The single-mineral chemical analysis results are shown in Table 1 and the X-ray diffraction spectrograms are shown in Figure 2.

Table 1. The multi-element chemical analysis results of single minerals (mass fraction, *wt%*).

Mineral	Mass Fraction/%							
	Mo	S	SiO ₂	MgO	Fe	CaO	Al ₂ O ₃	P
Molybdenite	57.09	38.14	4.32	-	0.12	0.10	0.22	-
Talc	-	-	67.03	31.73	0.59	0.47	0.12	0.024

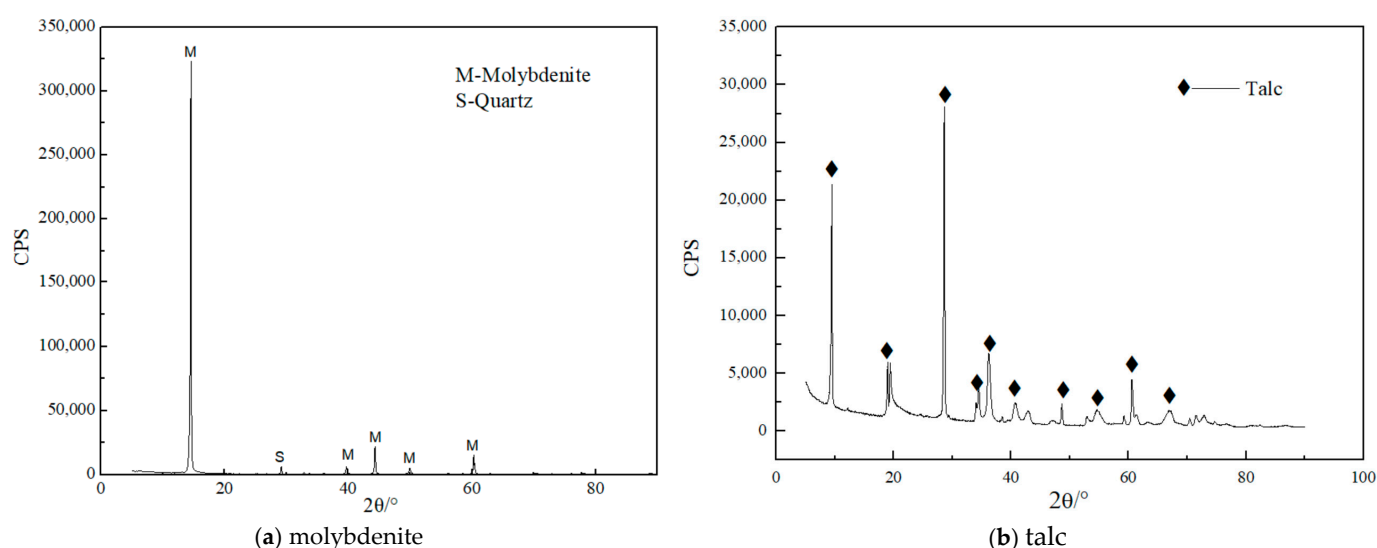


Figure 2. X-ray diffraction analysis of molybdenite (a) and talc (b) minerals.

The background electrolyte solution during the AFM measurement was 10 mM potassium chloride (KCl). The pH regulators were hydrochloric acid (HCl) and sodium hydroxide (NaOH) (analytical pure). The water used in the test was ultrapure water with a resistivity of 18.2 MΩ·cm.

2.2. Sample Cutting and Surface Treatments [20,21]

The mineral particle sample was cleaned by ultrasonic cleaning and dried with ultrapure nitrogen gas. First, we covered the bottom of the clean and dry molds with an A-B resin adhesive, which was prepared using a certain proportion. Secondly, we put the mineral particle sample in the molds when the A-B resin adhesive hardened after cooling for 3 to 4 h in a clean environment. Third, we covered the samples and filled the molds with an A-B resin adhesive without bubbles. Fourth, we took out the block from the molds after cooling for 4 h. Then, we cut the block with a slicer (Leica Microsystems Trading Co., Ltd., Shanghai, China) until the mineral was revealed. After that, further cutting using an

ultramicrotome(Leica Microsystems Trading Co., Ltd., Shanghai, China) was conducted to obtain a relatively smooth surface to meet the test requirements. Finally, the sample was stuck onto the metal substrate for analysis and measurements with an AFM (Bruker Technology Co., Ltd., Beijing, China). The scheme of sample preparation for this study is shown in Figure 3.

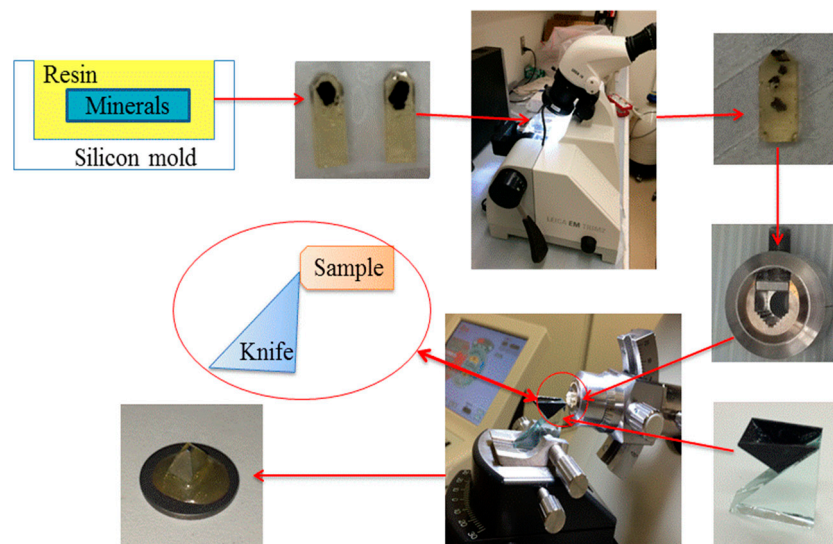


Figure 3. Diagrams showing the preparation of the mineral sample surfaces using the ultramicrotome cutting technique.

2.3. AFM Measurements

The spring constant of the cantilever used in the AFM was 0.07 to 0.15 N/m, and 10 mM potassium chloride (KCl) was supplied as the background electrolyte solution when measuring the samples in different pH values. Before the measurements, all the samples and the cantilevers were soaked in a solution with a specific pH to ensure the surfaces' purity. At each pH value, force measurements between the cantilever and sample were taken more than 5 times in different areas to ensure accuracy. All tests were performed at room temperature ($25 \pm 1^\circ\text{C}$).

2.4. Calculation of the DLVO Theoretical Model

The force between particles is the root of particle agglomeration and dispersion. It can be calculated using the DLVO theoretical model [22,23]:

$$F_T = F_W + F_E \quad (1)$$

Here, F_T is the force between particles. F_W is the van der Waals forces. F_E is the electrostatic force.

2.4.1. Van Der Waals Forces

Van der Waals forces are considered to be the major force that has always existed between macro objects. Van der Waals forces, which are related to the size and shape of the object, is the collection of the forces between the atoms or the molecules.

(1) The van der Waals energy between two spherical particles is

$$V_W = -\frac{AR_1R_2}{6H(R_1 + R_2)} \quad (2)$$

Here, R_1 and R_2 are the radius of the two particles, respectively. H is the distance between the particles. A is the Hamaker constant.

(2) The van der Waals energy between a platy particle and a spherical particle (R is its radius) is

$$V_W = -\frac{A}{6} \cdot \left(\frac{2R}{H} + \frac{2R}{H+4R} + \ln \frac{H}{H+4R} \right) \quad (3)$$

The van der Waals force is

$$F_W = -\frac{dV_W}{dH} \quad (4)$$

According to the formula, it can be deduced that van der Waals forces are not only related to the radius of particles but also the Hamaker constant. The Hamaker constant is actually an important parameter in the calculation of van der Waals forces. The Hamaker constants of the materials [24,25] referred to in this paper are shown in Table 2.

Table 2. Hamaker constants of materials in vacuum.

Materials	Water	Silicon Nitride	Silicon	Talc	Molybdenite
Hamaker constant/ $(\times 10^{-20} \text{ J})$	3.28	16.7	13.6	9.1	9.1

When A_{11} , A_{22} , and A_{33} are the Hamaker constants of materials 1 and 2 and medium 3, respectively, the Hamaker constant of the interactive potential energy between materials 1 and 2 when they are in medium 3 is

$$A_{132} = A_{12} + A_{33} - A_{13} - A_{23} \approx \left(\sqrt{A_{11}} - \sqrt{A_{33}} \right) \times \left(\sqrt{A_{22}} - \sqrt{A_{33}} \right) \quad (5)$$

2.4.2. Electrostatic Forces

Electrostatic forces are produced when the particles become close together and the electrostatic double layers begin to overlap. When the charges have the same sign, electrostatic forces appear as repulsive forces; otherwise, they appear as attractive forces. The electrostatic action of the same particles is often shown as a repulsive force, but if the surface of the same particles has a different charge, it may be shown as an attractive force. For dissimilar particles, an electrostatic action may be manifested as either a repulsive force or an attractive force, which is mainly determined by the surface charge of the particles.

1. Electrostatic energy between spherical particles with radius R and heterogeneous mineral plate particles:

$$V_E = \pi \varepsilon_r \varepsilon_0 R \left(\psi_1^2 + \psi_2^2 \right) \left[\frac{2\psi_1\psi_2}{\psi_1^2 + \psi_2^2} \ln \left[\frac{1 + \exp(-\kappa H)}{1 - \exp(-\kappa H)} \right] + \ln[1 - \exp(-2\kappa H)] \right] \quad (6)$$

2. Electrostatic energy of heterogeneous spherical particles with radii R_1 and R_2 :

$$V_E = \pi \varepsilon_r \varepsilon_0 \frac{R_1 R_2}{R_1 + R_2} \left(\psi_1^2 + \psi_2^2 \right) \left[\frac{2\psi_1\psi_2}{\psi_1^2 + \psi_2^2} \ln \left[\frac{1 + \exp(-\kappa H)}{1 - \exp(-\kappa H)} \right] + \ln[1 - \exp(-2\kappa H)] \right] \quad (7)$$

The electrostatic force is:

$$F_E = -\frac{dV_E}{dH} \quad (8)$$

V_E is the electrostatic potential energy per unit area, J/m^2 ; ε_r is the dielectric constant of water, 78.5; ε_0 is the absolute dielectric constant in vacuum, $8.854 \times 10^{-12} \text{ C}^{-2} \cdot \text{J}^{-1} \cdot \text{m}^{-1}$;

and ψ is the surface potential of the mineral V , which can be replaced by the Zeta potential. H is the distance between particles, m; k is the Boltzmann constant, 1.38×10^{-23} J/K; and κ^{-1} is the Debye length, m, calculated to be 0.104 nm. F_W is the electrostatic force per unit area, N/m².

2.5. Calculation of Adsorption Energy

The adsorption energies of water (H₂O) and nitrogen (N₂) on mineral surfaces are calculated as shown in [26]:

$$E_{\text{ads}} = E_{\text{x/surface}} - E_{\text{x}} - E_{\text{surface}} \quad (9)$$

where E_{ads} is the adsorption energy; E_{x} is the energy of the H₂O or N₂ molecules calculated in a cubic cell ($x = \text{H}_2\text{O}$ or N_2); E_{surface} is the energy of the molybdenite or talc slab; and $E_{\text{x/surface}}$ is the energy of the talc or molybdenite slab with adsorbed H₂O and N₂.

2.6. Floatation Experiment

Single-mineral floatation was measured using a floatator (XFG-60 type, Wuhan Exploration Machinery Co., LTD, Wuhan, China) [27]. The spindle speed is 1650 r/min. We put 3.0 g of the mineral (particle size $\leq 100 \mu\text{m}$) in the 40 mL floatation cells every time, added 30 mL of distilled water, and mixed for 1 min. Then, we adjusted the pH with hydrochloric acid or sodium hydroxide solution, stably stirred for 2 min, and detected the pH. We successively added the inhibitor, collector, and frother, and mixed the pulp for 3 min, respectively. The floatation time was 4 min. We dried and weighed the bubble products and slot products separately and calculated the recovery.

3. Results and Discussion

3.1. Adsorption Energy of Water Molecules on Different Crystal Planes of Molybdenite and Talc [28–31]

We simulated and calculated the adsorption of water molecules on different surfaces of molybdenite and talc to study the hydrophobic properties of the crystal surfaces. The Castep module based on density functional theory and the plane wave pseudopotential method in Materials Studio 7.0 (MS) software was used for this calculation. In this work, all calculations were carried out in a vacuum environment to completely eliminate the effects of oxygen and other similar factors.

Figure 4 shows the optimized adsorption model of water molecules on the surfaces of molybdenite and talc crystals. Table 3 shows the distance changes between O atoms and metal atoms on the mineral surfaces after adsorption of the water molecule, where r_0 is the radius of oxygen atoms in the water molecule, r_e is the radius of metal atoms, d_0 is the sum of the radii between oxygen atoms and metal atoms, d_{ads} is the distance between oxygen atoms and mineral metal atoms in the water molecule after adsorption, and Δd is the difference between d_{ads} and d_0 .

Table 3. Variations of the distance between the O atoms of H₂O and the metal atoms of mineral surfaces.

Mineral	$d_0 (=r_0 + r_e)/\text{\AA}$	$d_{\text{ads}}/\text{\AA}$	$\Delta d (=d_{\text{ads}} - d_0)/\text{\AA}$
Molybdenite	2.05	3.962	1.912
Talc	2.10	3.276	1.176

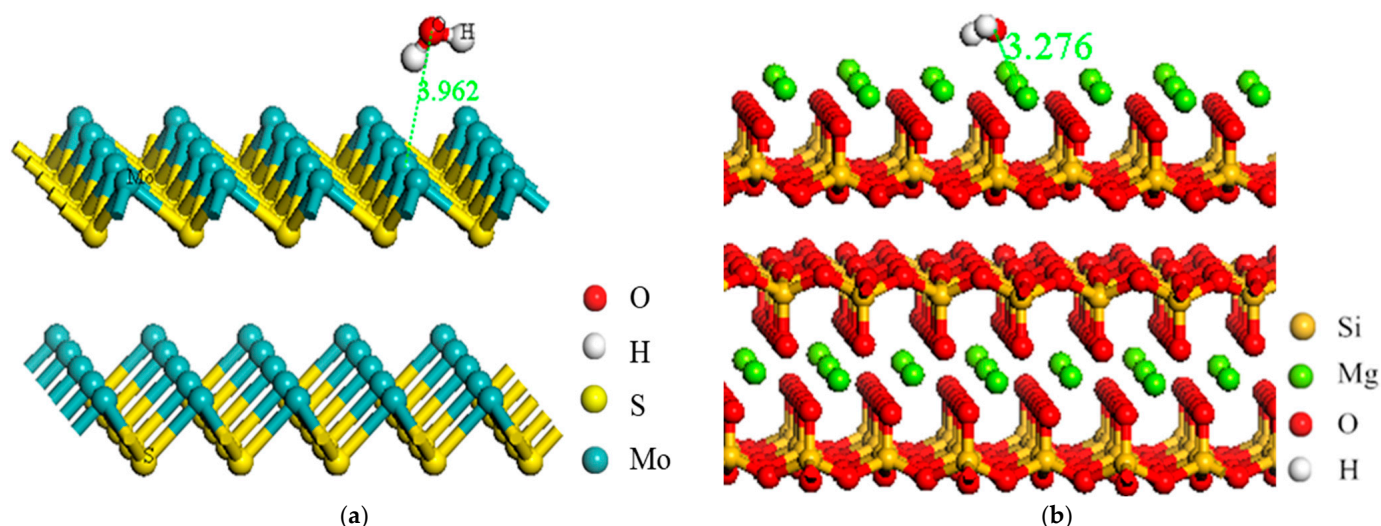


Figure 4. Adsorption models of H₂O molecules on molybdenite (a) and talc (b) surfaces.

It can be seen that the Δd values of molybdenite and talc are 1.912 Å and 1.176 Å, respectively, which are both greater than zero. It indicates that there is no reaction between water molecules and the mineral after optimization. The water molecules still exist in water instead of on the mineral surfaces, which proves that it is difficult to adsorb water molecules onto the surface of molybdenite or talc.

Table 4 shows the adsorption energies of H₂O molecules on different crystal faces of molybdenite and talc, where $E_{\text{H}_2\text{O-mineral}}$ is the interaction energy between mineral and water molecules after adsorption, $E_{\text{H}_2\text{O-H}_2\text{O}}$ is the interaction energy between water molecules, and ΔE is the difference between $E_{\text{H}_2\text{O-mineral}}$ and $E_{\text{H}_2\text{O-H}_2\text{O}}$. A negative sign represents an exothermic reaction. The data reveal that the adsorption energy of H₂O on the molybdenite crystal faces (103) is the largest at −24.42 kJ/mol; whereas that on the crystal faces (001) is the smallest at −10.59 kJ/mol. The adsorption energy of H₂O on the talc crystal faces (100) is the largest at −3.46 kJ/mol; whereas that on the crystal faces (001) is the smallest at −0.20 kJ/mol. The data comparison shows that the (001) surfaces of both talc and molybdenite have the lowest negative values, indicating that the (001) surface is the most difficult for water molecules to interact with among all crystal surfaces. Talc is more hydrophobic than molybdenite. In fact, interactions also exist between H₂O molecules, affecting the adsorption of H₂O molecules toward the mineral surfaces. The binding energy between H₂O molecules ($E_{\text{H}_2\text{O-H}_2\text{O}}$) was calculated to be −21.94 kJ/mol. The smaller the interaction energy between substances, the more stable the substance is in this state. It indicates that water molecules can interact with minerals more easily when $\Delta E < 0$. On the contrary, the water molecules can interact with each other when $\Delta E > 0$, while the larger the value of ΔE , the stronger the hydrophobicity. These results suggest that H₂O molecules prefer to stay with the crystal faces (103) at the edge surface rather than the crystal faces (001) at the basal surface.

Table 4. Adsorption energies of H₂O molecules on the different crystal faces of minerals.

Minerals	Crystal Surface	Adsorption Energy/(kJ/mol)		
		$E_{\text{H}_2\text{O-mineral}}$	$E_{\text{H}_2\text{O-H}_2\text{O}}$	$\Delta E = E_{\text{H}_2\text{O-mineral}} - E_{\text{H}_2\text{O-H}_2\text{O}}$
Molybdenite	(001)	−10.59	−21.94	11.35
	(100)	−14.14	−21.94	7.80
	(010)	−12.13	−21.94	9.81
	(101)	−17.65	−21.94	4.29
	(103)	−24.42	−21.94	−2.48
	(112)	−14.54	−21.94	7.40
	(110)	−15.88	−21.94	6.06
Talc	(001)	−0.20	−21.94	21.74
	(100)	−3.46	−21.94	18.48
	(010)	−1.48	−21.94	20.46
	(101)	−2.27	−21.94	19.67
	(103)	−0.78	−21.94	21.16

3.2. The Calculated Stern Potential of Different Crystal Planes

Studies have shown that the electrification of the mineral basal planes and edge surfaces are different. The stern potential of the basal and edge surfaces is studied through AFM and the DLVO theory in this work.

3.2.1. The Surface Potential Values of Silicon Nitride

Firstly, the zeta potential of the silicon nitride probe was calculated by measuring and fitting the AFM force curve (the Zeta potential was considered to be approximately equal to the stern potential in this paper, which is the same as below). As shown in Figure 5, when the pH was 3.5, 5.5, 7.5, and 9.5, the Zeta potential of the silicon nitride was 14 mV, −38 mV, −48 mV, and −56 mV, respectively. The other three curves are the silicon nitride potential obtained by other scholars or studies in the literature using electrolyte solutions of different concentrations or types [32,33].

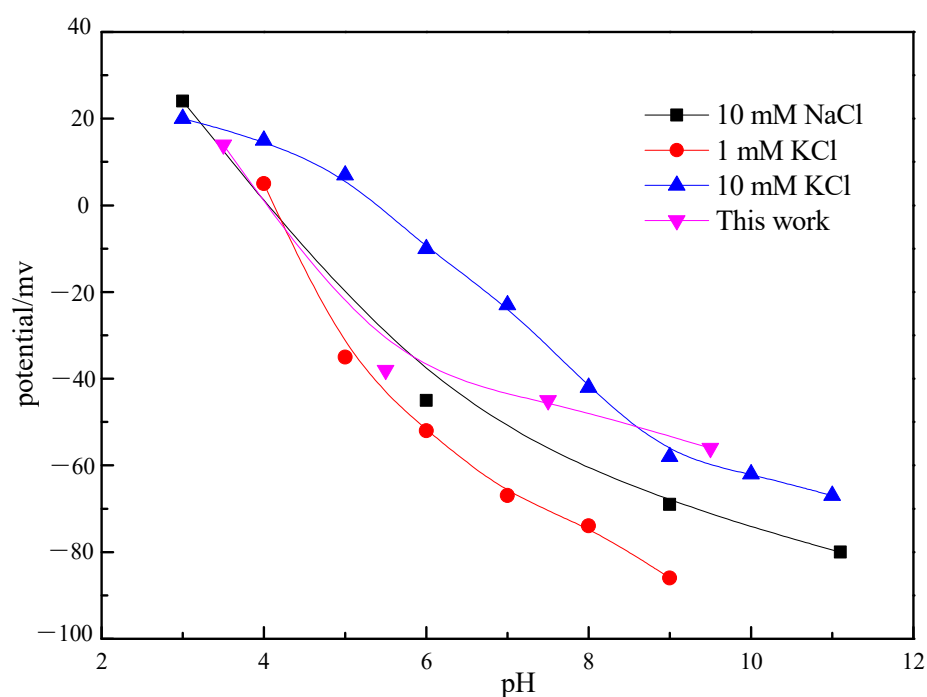


Figure 5. Comparison of the surface potential values of silicon nitride.

3.2.2. AFM Force Curves [34,35]

AFM scanning was performed on the prepared molybdenite and talc samples. The non-polar (plane) surface of molybdenite is very smooth, with a roughness of 1.732 nm. The polar (edge) surface of molybdenite is banded, with a roughness of 2.234 nm. The non-polar (plane) surface of talc is also very smooth, with a roughness of 1.518 nm, and the polar (edge) surface has a roughness of 2.132 nm. Both areas meet the requirements for AFM force curve measurements.

AFM force curves were measured and analyzed for the required samples, and the force action curves between non-polar and polar surfaces of silicon nitride and molybdenite were obtained at different pH values, as shown in Figure 6.

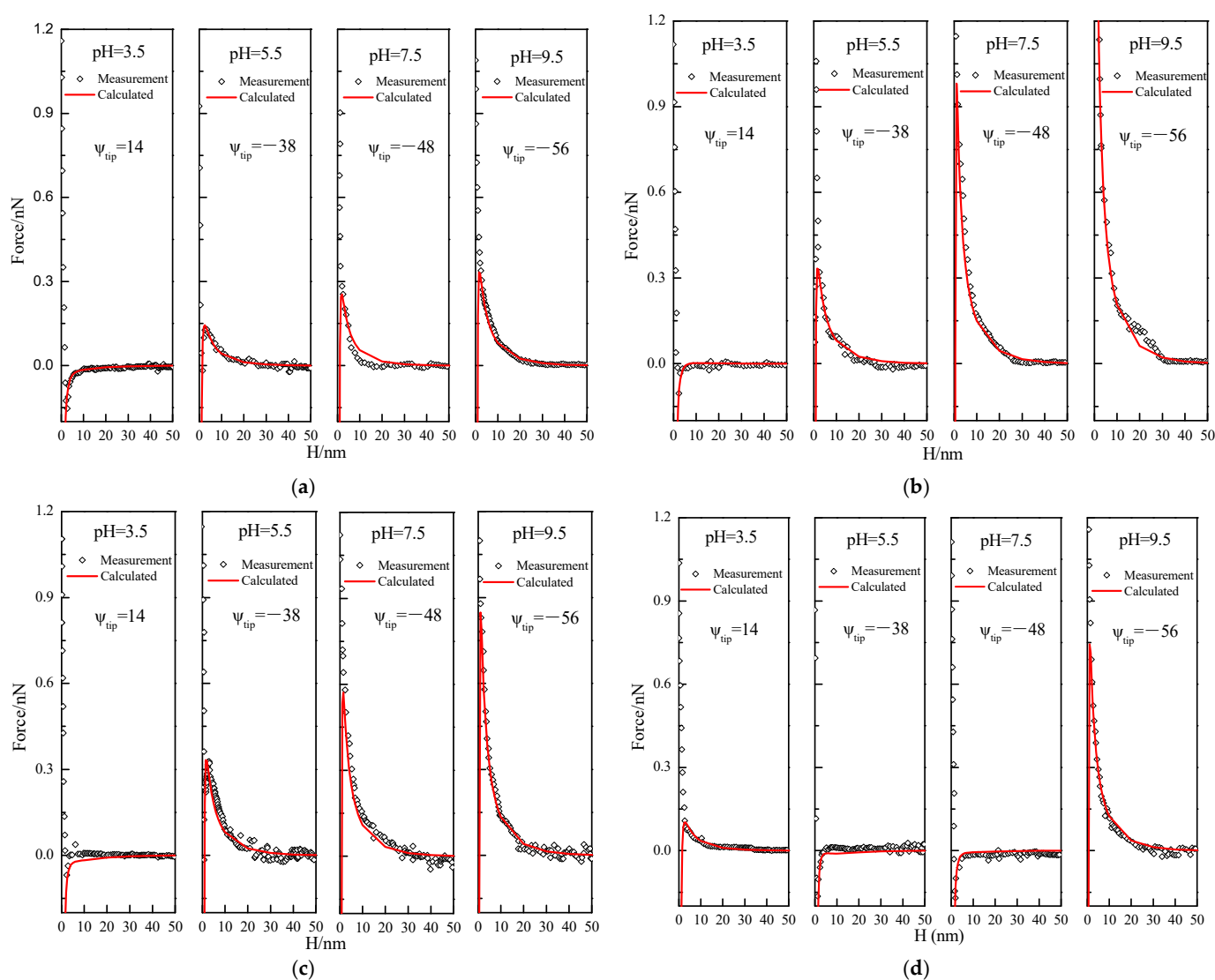


Figure 6. Force profiles calculated and measured between the AFM tip and molybdenite basal plane (a); molybdenite edge surface (b); talc basal plane (c); and talc edge surface (d) at different pH values.

As can be seen from Figure 6, with the increase in pH values, the attraction between the molybdenite polar plane and silicon nitride becomes weaker while the repulsion becomes stronger. When the pH is 3.5, there is attraction between molybdenite's non-polar plane and silicon nitride. When the pH value increases, the force is shown as a repulsive force. With the increase in pH values, the force becomes larger. Talc has the same experimental

results as molybdenite. In addition, it can be seen from the figure that the calculated values are basically consistent with the measured values.

3.2.3. The Calculated Zeta Potential Values of Different Crystal Planes

According to the DLVO theory, all parameters except the potential value are known. Therefore, the zeta potential values of the non-polar and polar surfaces of molybdenite and talc can be obtained by fitting the force curve measured by AFM, as shown in Figure 7. As can be seen in Figure 7, the potential values of the non-polar planes of molybdenite and talc are relatively constant and are basically not affected by the environmental pH value. The potential values of the non-polar planes are both negative, which is caused by the lattice defect or lattice substitution in the crystal structure of molybdenite or talc. The potential value of the polar plane decreased with the increase in pH, and the zero point of molybdenite's polar plane is at a pH of 3.8, while the zero point of talc's polar plane is at a pH of 7.6.

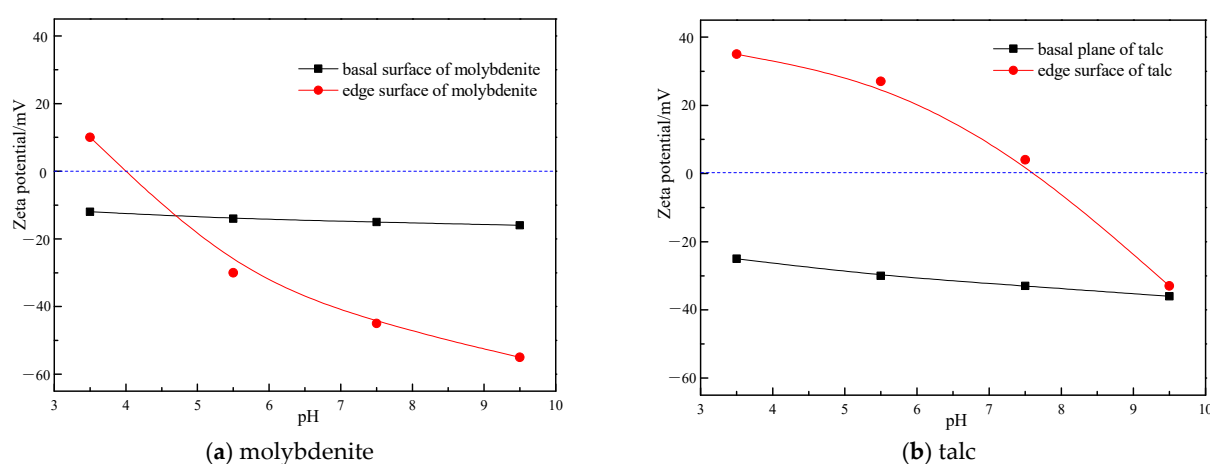


Figure 7. The calculated zeta potential values of mineral basal and edge surfaces.

3.3. The Force Profiles Between Different Crystal Planes

The zeta potential values of mineral basal and edge surfaces have been obtained under different pH conditions. Therefore, we can calculate the interaction force between the faces of molybdenite and talc, as shown in Figure 8.

The results show that the force between the molybdenite basal plane and the talc basal plane has always been exclusive within the experimental pH range. The force between the molybdenite basal plane and the talc edge surface is exclusive between pH levels of 8.5 and 9.5, while they attract each other at pH levels of 7.5, 5.5, and 3.5. The force between the molybdenite edge surface and the talc basal plane is exclusive, except at a pH of 3.5. The force between molybdenite and the talc edge surface is exclusive at pH levels of 8.5, 9.5, and 3.5, while they attract each other at pH levels of 5.5 and 7.5. In summary, the interaction force between molybdenite and talc is exclusive only at pH levels ≥ 8.5 . Therefore, it is best to choose the floatation separation of talc and molybdenite in an alkaline environment.

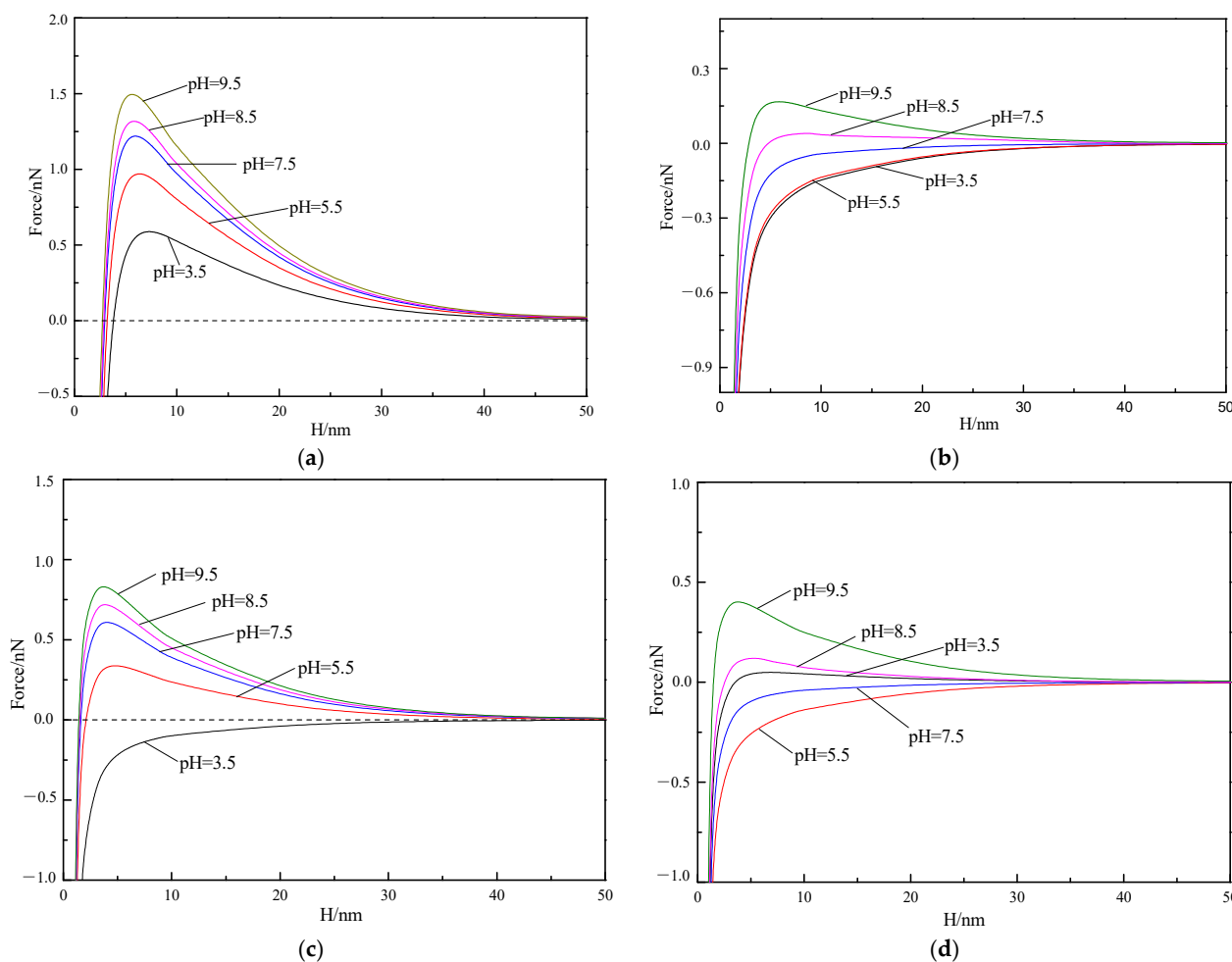


Figure 8. The force profiles calculated between the molybdenite basal plane and the talc basal plane (a); the molybdenite basal plane and talc edge surface (b); the molybdenite edge surface and talc basal plane (c); and the molybdenite edge surface and talc edge surface (d).

3.4. Effect of Crystal Surface Anisotropy on Flotation Behavior

The flotation tests of single minerals and artificial mixed minerals (the mass ratio of molybdenite and talc is 1:5) at different pH values are studied to verify the effect of crystal surface anisotropy on flotation separation, as shown in Figure 9. The flotation experiments were performed in accordance with the methodology outlined in Section 2.6. Prior to flotation, the pulp pH was precisely adjusted to the target value using NaOH/HCl solutions and allowed to stabilize for 2 min. The collector sodium butyl xanthate (20 g/t), inhibitor CMC (40 g/t), and frother MIBC (10 g/t) were then sequentially introduced with 2 min conditioning periods between additions. Flotation was initiated by air injection at a fixed rate of 0.3 L/min for 4 min of collection time.

The flotation results demonstrate distinct pH-dependent recovery patterns for molybdenite and talc (Figure 9). Single mineral flotation tests revealed that molybdenite maintained consistently high recovery (>72%) across the entire experimental pH range (3–10), while talc showed characteristically low recovery (<30%) under all conditions. However, in artificial mixed mineral flotation tests, a significant trend emerged: talc recovery progressively decreased from 57% to 32% as pH increased from 3 to 10, meanwhile molybdenite recovery progressively increased from 52% to 63%, suggesting pH-mediated interparticle interactions between the two minerals.

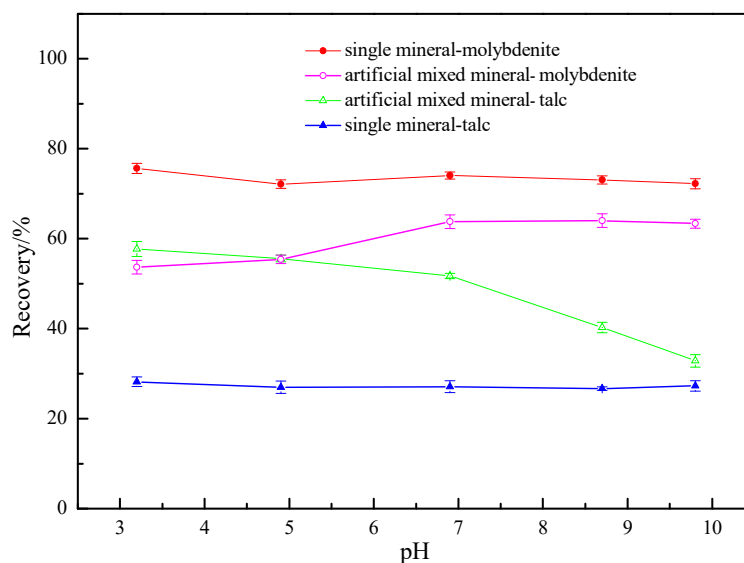


Figure 9. The floatation tests of single minerals and artificial mixed minerals at different pH values.

This behavior can be attributed to the changing interfacial chemistry between molybdenite and talc particles. As shown in Figure 10, EDS analysis (points a-1 and a-2) confirms extensive hetero-aggregation at a pH of 5.21, with fine talc particles (Mg/Si-rich) adhering to larger molybdenite surfaces (Mo/S-rich). The aggregation intensity weakened at a pH of 7.17 (Figure 10b), and complete dispersion occurred in alkaline conditions (pH > 9). These observations align with our DLVO calculations (Section 3.3). In acidic/neutral conditions (pH 3–7), electrostatic attraction between positively charged talc edges ($\text{Si-O}^-/\text{Mg-OH}_2^+$) and negatively charged molybdenite basal planes promoted aggregation, enhancing talc recovery. Under alkaline conditions, both minerals developed strong negative surface charges, creating repulsive forces that improved dispersion. This selective dispersion enabled effective molybdenite floatation while depressing talc, with optimal separation achieved at a pH of 9.0. These findings provide both technical guidance and a theoretical foundation for industrial separation processes.

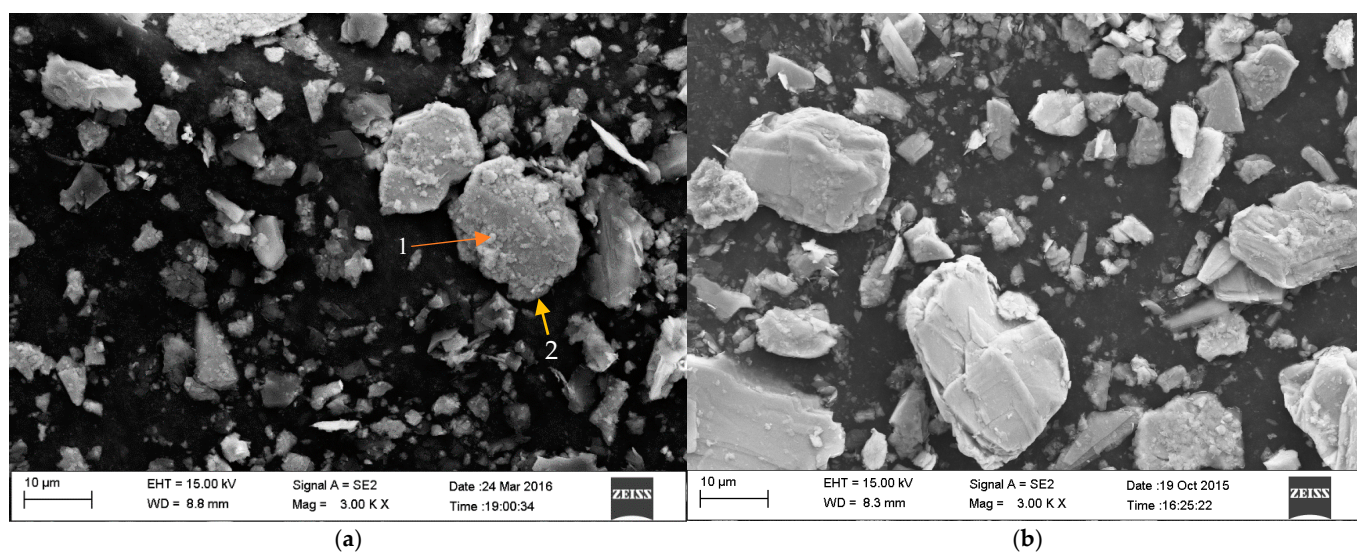


Figure 10. Cont.

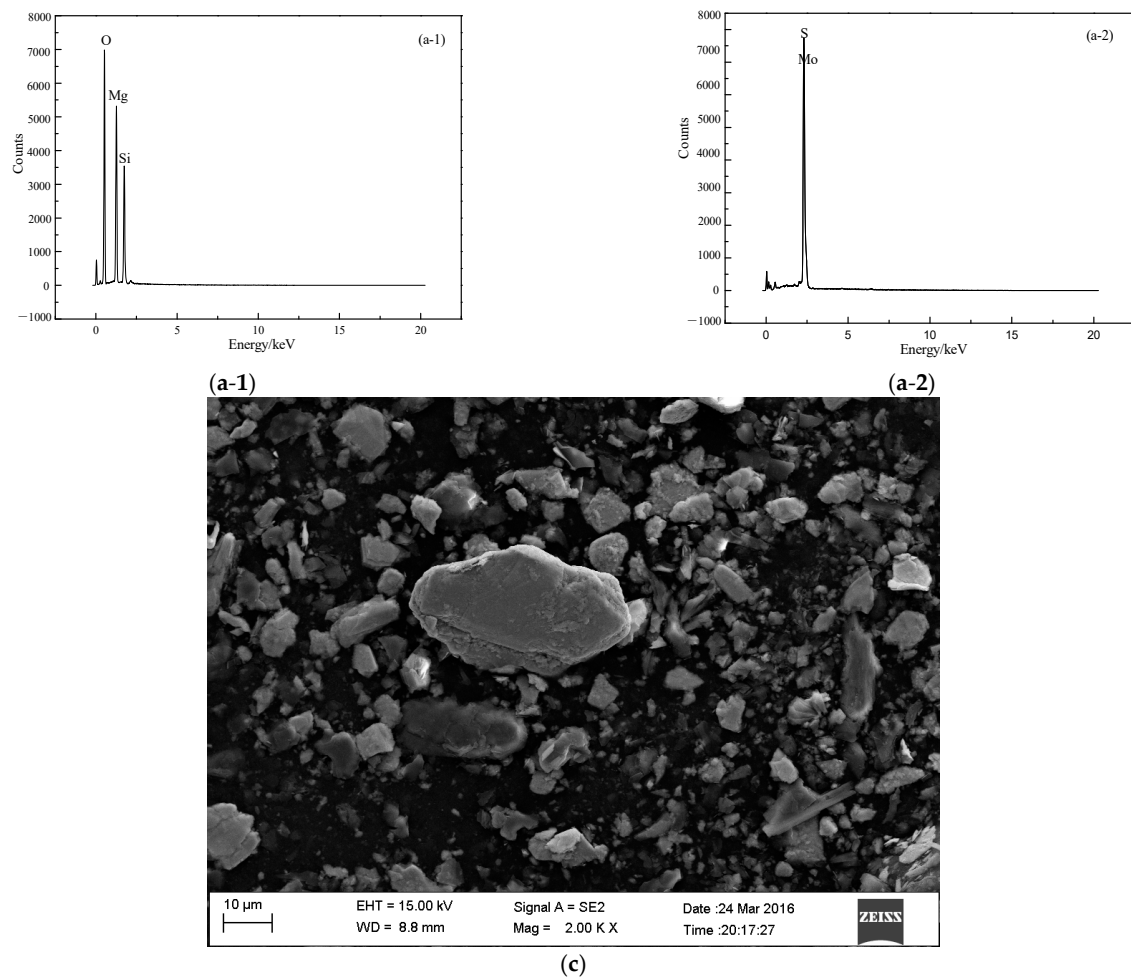


Figure 10. The SEM photographs of concentrates for artificial mixed minerals under different pH values: pH = 5.21 (a); pH = 7.17 (b); pH = 9.13 (c); (a-1): EDS spectra analysis of point 1; (a-2): EDS spectra analysis of point 2.

4. Conclusions

1. Density functional theory (DFT) calculations revealed that the basal planes of both molybdenite and talc exhibit strong hydrophobicity, while their edge surfaces are hydrophilic. The adsorption energy of water molecules on the basal planes was significantly lower than on edge surfaces, confirming the intrinsic hydrophobic nature of these planes. Notably, talc demonstrated even greater hydrophobicity than molybdenite, which complicates their separation during floatation.
2. Atomic force microscopy (AFM) and DLVO theory analyses demonstrated that the surface potential of the non-polar basal planes remains relatively constant and negative across a wide pH range, attributed to lattice defects or substitutions. In contrast, the polar edge surfaces exhibited pH-dependent behavior, with the point of zero charge (PZC) occurring at pH 3.8 for molybdenite and pH 7.6 for talc. This divergence in surface charge under varying pH conditions critically influences interparticle interactions.
3. This study identified that hetero-aggregation between molybdenite and talc is prevalent in neutral or acidic conditions due to electrostatic attraction between oppositely charged surfaces. However, under alkaline conditions (pH > 8.5), strong repulsive forces between negatively charged surfaces promote particle dispersion. This pH-mediated behavior is pivotal for achieving selective floatation.

4. Flotation experiments validated these theoretical insights, showing that alkaline conditions (pH ~ 9.0) significantly reduce talc recovery while enhancing molybdenite recovery. The dispersion of particles at high pH minimizes unwanted hetero-aggregation, enabling efficient separation. SEM-EDS analysis further corroborated these results, revealing a clear reduction in talc–molybdenite aggregation at an alkaline pH.

In conclusion, this work elucidates the fundamental mechanisms governing the floatation separation of molybdenite and talc, offering a scientifically grounded strategy for optimizing industrial practices. The integration of DFT, AFM, and DLVO theory provides a robust framework for understanding and manipulating surface interactions in mineral processing, with potential applications extending to other challenging separations involving anisotropic minerals. Future research could explore the role of advanced reagents or alternative pH modifiers to further enhance selectivity and recovery.

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