

Article

Study on the Galvanic Interaction of Gold and Main Associated Minerals Based on Density Functional Theory

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Abstract: The galvanic interaction of gold and associated sulfide minerals in thiocyanate systems has a significant impact on gold leaching. The density functional theory was used to further reveal the galvanic interaction between gold and associated minerals. The electron transfer between gold and its associated minerals at different galvanic interaction distances was simulated. The results show that with the increase of the contact distance between pyrite and gold, the charge of pyrite increases, indicating that it is losing electrons gradually; the charge of arsenopyrite and chalcocite decreases with the rise of the contact distance between gold and pyrite, suggesting that they are gaining electrons. In addition, gold has the greatest influence on the gain and loss of electrons in pyrite and arsenopyrite and has the least influence on chalcocite. Through the calculation of the density of states, it is found that different distances of galvanic interaction have a great influence on the density of states of surface atoms under the action of pyrite and arsenopyrite with gold but have little effect on the density of states of surface atoms under the action of chalcocite with gold.

Keywords: gold leaching; associated sulfide minerals; galvanic interaction; density functional theory



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1. Introduction

Gold is a particular metal that provides national financial security. In the metallurgical process, leaching is the main means of extracting gold. Currently, the main leaching agent used for gold leaching is cyanide. However, due to its high toxicity and serious environmental pollution, scholars have developed a variety of less toxic leaching agents to replace cyanide in recent years. Environmentally friendly gold leaching agents include thiosulfate, stone sulfur agents, thiourea, thiocyanates, etc. [1–3]. Among many environmentally friendly gold leaching agents, thiocyanate gold leaching agents have attracted more attention due to the advantages of high efficiency, low toxicity, and environmental protection. SCN[−] ions in thiocyanate gold leaching agents have a strong ability to form complexes with Au (I) and Au (III), and the gold leaching efficiency is close to that of cyanide. At the same time, the toxicity is only 1.17% of that of cyanide [4–6].

Gold concentrates are associated with a considerable amount of sulfide minerals, such as a gold mine in Ethiopia. The gold concentrate produced contains galena, sphalerite, and copper sulfide minerals, with monomer gold and fissure gold accounting for 93% [7]. In addition, common associated minerals of gold include chalcocite, stibnite, quartz, feldspar, and so on. The thiocyanate gold leaching system is a complex electrochemical system, in which electron transfer occurs not only between the gold leaching agent and gold but also between different sulfide minerals. When the conductor or semiconductor material in electrical contact state is in the leaching system, a galvanic cell will occur. The metal corrosion caused by the galvanic interaction is called galvanic corrosion [8–10]. Galvanic interaction can enhance the corrosion of one or more substances and the cathodic protection of other substances in an electrochemically coupled mineral system. Substances with a lower electrostatic potential undergo an anodic reaction, while minerals with a higher electrostatic potential undergo cathodic passivation. The electrostatic potential of sulfides is related to their Fermi level. When two minerals come into contact, electrons flow from minerals with high Fermi levels to minerals with low Fermi levels, until the two minerals have the same Fermi level, reaching equilibrium. The driving force of the galvanic interaction between sulfide minerals is precisely due to the difference in the electron Fermi energy levels between the two minerals. The greater the difference in Fermi energy levels between the two minerals, the more significant their galvanic interaction is [11,12]. Therefore, it is of great significance to study the influence of associated minerals on gold leaching.

In the cyanide leaching system of gold, some scholars have studied the effect of the galvanic interaction between sulfide minerals and gold on gold leaching. M.M. Aghamirian [9] believed that in the cyanide leaching system of gold, the electric couple composed of chalcopyrite, chalcocite, and gold has an inhibiting effect on the dissolution of gold, while the electric couple composed of pyrite, pyrrhotite, galena, and gold has a promoting effect on the dissolution of gold. In the thiocyanate system, M. Sadigh Safarzadeh [13] studied the stability of several sulfide minerals in the acidic thiocyanate system and found that the dissolution situation was as follows: chalcocite, bornite > copper blue, sulfur arsenic steel ore > pyrite, chalcopyrite. It can be seen that the dissolution behavior of associated minerals in the thiocyanate system and its influence on the thiocyanate system has attracted the attention of researchers. However, there are few studies on the effect of the dissolution behavior of associated minerals on gold dissolution based on the physical properties of mineral solids.

With the increasing maturity of quantum mechanical computing methods, using density functional theory (DFT) to simulate complex topics in minerals has received increasing attention. Wu Biao [14] adopted a first principles approach based on density functional theory to study the electronic structures and properties of three sulfide minerals, pyrite, chalcocite, and copper blue, at the atomic and molecular levels, revealing the dissolution differences of the three sulfide minerals from the microscopic essence, laying a theoretical foundation for achieving selective leaching. Darius Azizi [15] and others have revealed some important electronic characteristics of gold and pyrite during the cyanidation process through density functional theory simulations. Studies have shown that the preferential adsorption of cyanide on the gold surface is caused by current interaction or oxidation of gold, resulting in a higher electron deficiency of gold than at the pyrite site. As the electron deficiency in the Au atom increases, the interaction between gold and CN^- will increase, thereby promoting the dissolution of gold. Therefore, based on the physical properties of mineral solids, starting with the solid energy band structure, crystal structure, and surface structure of associated minerals of gold is the basis for studying the electrochemical interaction between associated minerals and gold in thiocyanate systems.

In this work, within the framework of density functional theory, using the CASTEP modules in Material Studio software, the crystal cell structures of gold and typical associated minerals were established. On this basis, the electron transfer during the galvanic interaction between gold and associated minerals, and the density of states of pyrite, ar-

senopyrite, chalcocite, and gold surface were studied. Thus, the relationship between gold and associated minerals under the galvanic interaction is expounded.

2. Method and Model

Based on density functional theory, all calculations are completed using the CASTEP module [16]. The commutative correlation functional uses the PBE functional under the generalized gradient approximation (GGA) [17]. The interaction between valence electrons and ionic realms is described using super soft pseudopotentials. The plane wave cutoff energy is selected as 600 eV. The energy of the model is calculated. All calculation models are calculated using a $1 \times 1 \times 1$ Monkhorst-Pack point [18–20]. Spin polarization is considered in the calculation process.

The slab-slab model can well simulate the solid–solid interface problems [21,22]. In this paper, the slab-slab model is used to study the galvanic interaction between pyrite and gold, arsenopyrite and gold, and chalcocite and gold surfaces. The layered crystal to layered crystal surface contact model of pyrite and gold, arsenopyrite and gold, and chalcocite and gold is shown in Figures 1–4. The optimized layered crystal surface of pyrite (100), arsenopyrite (110), and chalcocite (110) are combined with the layered crystal surface of gold (100) using the build layer tool.

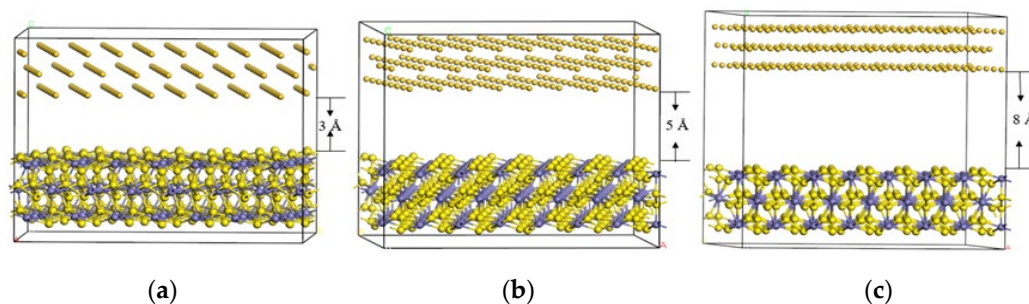


Figure 1. Galvanic interaction at different contact distances (a) 3 Å, (b) 5 Å, (c) 8 Å between pyrite and gold.

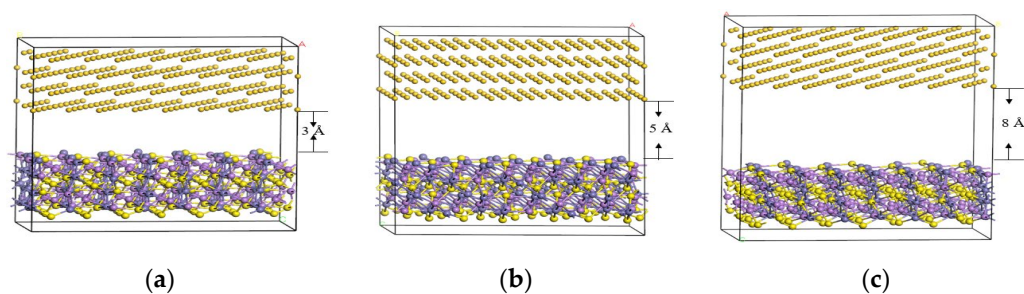


Figure 2. Galvanic interaction of different contact distances (a) 3 Å, (b) 5 Å, (c) 8 Å between arsenopyrite and gold.

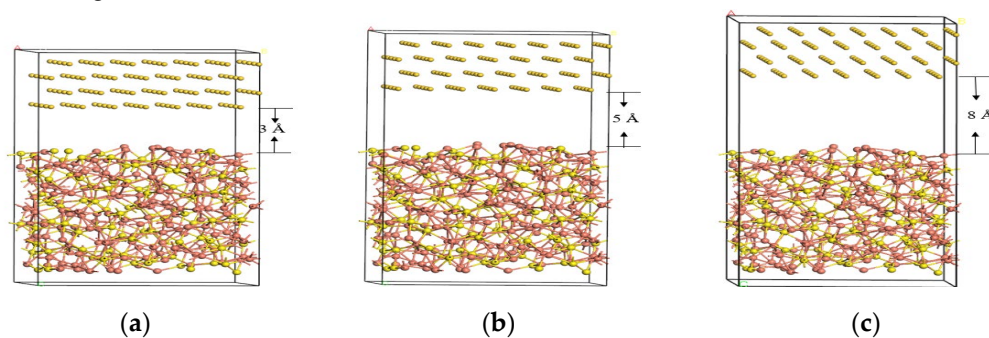


Figure 3. Galvanic interaction at different contact distances (a) 3 Å, (b) 5 Å, (c) 8 Å between chalcocite and gold.

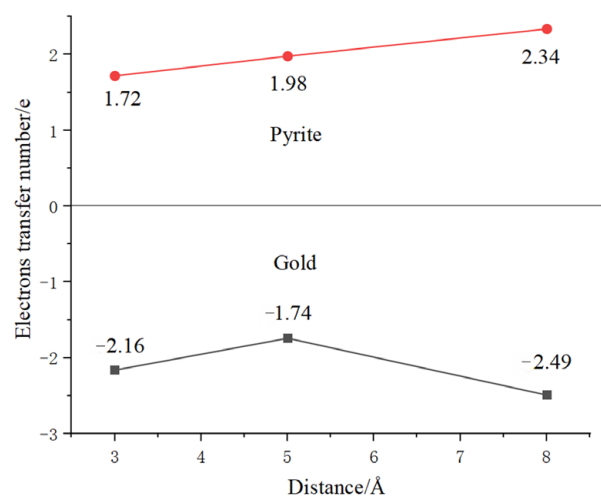


Figure 4. Effect of different galvanic interaction distances on the charge of pyrite and gold.

In order to achieve a better matching ratio between the mineral and gold surface and better combination, a larger mineral and gold supercell surface was used. In Figure 1, $a = 26.84 \text{ Å}$, $b = 26.84 \text{ Å}$ are the unit cell parameters of the pyrite and gold model. The model consists of a 9-layer pyrite (100) surface and a 3-layer gold (100) surface. In Figure 2, $a = 24.28 \text{ Å}$, $b = 26.28 \text{ Å}$ are the unit cell parameters of the arsenopyrite and gold model. The model includes a 16-layer atomic layer of arsenopyrite (110) surface and a 4-layer atomic layer of gold (100) surface. In Figure 3, $a = 14.12 \text{ Å}$, $b = 20.05 \text{ Å}$ are the unit cell parameters of the chalcocite and gold model.

In order to study the galvanic interaction between pyrite, arsenopyrite, and chalcocite and gold, we adjusted and changed the distance between the mineral and the surface of the gold stratiform crystal and established a galvanic interaction model with different distances (3 Å, 5 Å, 8 Å) between the mineral and the surface of the gold stratiform crystal, as shown in Figures 1–3.

3. Results and Discussion

3.1. Electron Transfer in the Process of Galvanic Interaction between Gold and Associated Mineral

In order to explain the galvanic interaction between gold and associated sulfide minerals in the thiocyanate system at the atomic and molecular levels, the electron transfer in this process was simulated by density functional theory.

Figures 4–6 show the effects of different galvanic interaction distances (3 Å, 5 Å, 8 Å) on the charge between pyrite, arsenopyrite, and chalcocite and gold after interaction. As shown in Figure 4, after the galvanic interaction, the charge of pyrite stratiform crystals is positive while the charge of gold stratiform crystals is negative. And, the charge of pyrite increases as the distance between the two layers of crystals increases, indicating that pyrite gradually loses electrons as the distance increases. The study of Tafel curve by Le et al. [23] showed that the corrosion potential of pyrite was lower than that of gold, and pyrite was oxidized as an anode to lose electrons. When the distance between the charges of gold is 8 Å, the charge is the most negative and the number of electrons obtained by gold is the highest.

Figure 5 shows the effect of different galvanic interaction distances (3 Å, 5 Å, 8 Å) on the charge between arsenopyrite and gold after galvanic interaction. As shown in the figure, the charge of the arsenopyrite layer crystal is positive and decreases with the increase of the action distance, indicating that the arsenopyrite gradually gains electrons with the increase of the distance. The charge of gold is negative and increases with distance, indicating that gold gradually loses electrons as distance increases. The results of Tafel curve also show that arsenopyrite can be used as a cathode to promote the dissolution of gold [23]. The

electron numbers of arsenopyrite and gold are close, and as the contact distance changes, the number of electrons gained/lost by arsenopyrite and gold is also relatively close.

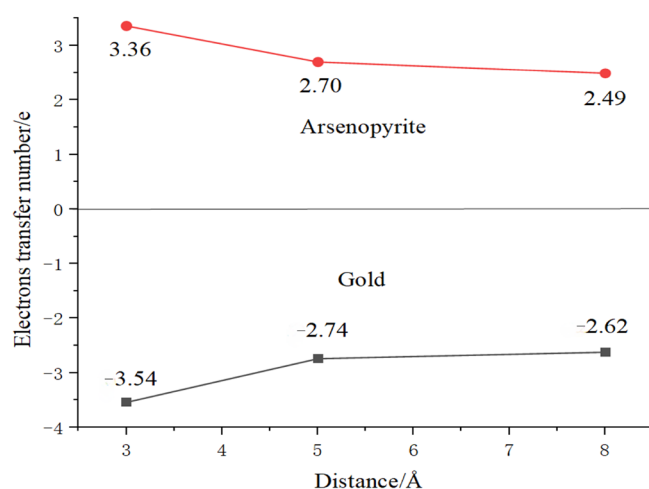


Figure 5. Effect of different galvanic interaction distances on the charge of arsenopyrite and gold.

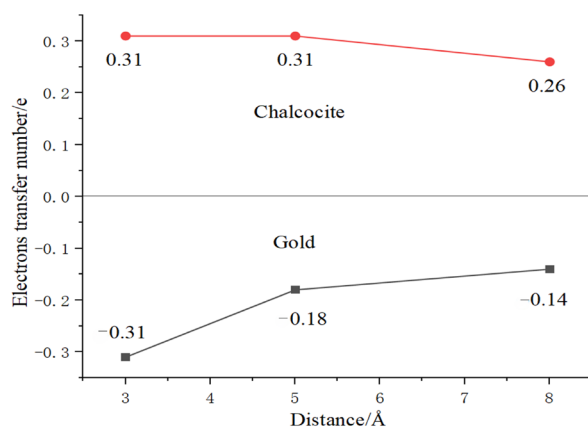


Figure 6. Effect of different galvanic interaction distances on the charge of chalcocite and gold.

Figure 6 shows the effect of different galvanic interaction distances (3 Å, 5 Å, 8 Å) on the charge between chalcocite and gold after galvanic interaction. As shown in the figure, the charge of chalcocite stratiform crystals is positive after gavage treatment, and slightly decreases with the increase of the treatment distance, indicating that chalcocite gradually gains electrons with the increase of the treatment distance. The charge of gold is negative and increases with distance, indicating that gold gradually loses electrons as distance increases. Under different action distances, the charge of chalcocite has almost no change, indicating that gold has the smallest effect on the gain and loss of electrons in chalcocite under the galvanic interaction.

It is found that under the influence of different galvanic interaction distances on the interaction model of pyrite, arsenopyrite, and chalcocite with gold, the charge number of pyrite increases with the increase of distance, indicating that pyrite loses electrons and inhibits the dissolution of gold. As the distance increases, the charge number of arsenopyrite and chalcocite decreases, indicating that arsenopyrite and chalcocite obtain electrons and promote gold dissolution. Moreover, gold has the greatest impact on the gain and loss of electrons in pyrite and arsenopyrite, and the smallest impact on chalcocite.

3.2. Effect of Galvanic Interaction on the Surface Properties of Gold and Associated Minerals

Galvanic interaction has a great influence on the surface properties of pyrite, arsenopyrite, and chalcocite with gold. Figure 7 shows the density of states of the Fe 3s, 3p, 4s, 3s, 3s,

5s, and 3d of the Au 6s, 5p, and 5d near the Fermi level (set the energy at 0 eV is the Fermi level). From Figure 7, Fe 3d, 3p, 4s and S Fe 3s, 3p states change less at contact distances of 3 Å and 5 Å, only at about 5 eV, and the density of Fe 3p and S 3p states increases with increasing distance; it shows that the atom has high reactivity. However, when the contact distance is 8 Å, the 3p, 4s and S 3p and 3s orbit of Fe have significant changes. At about 7 eV, Fe 3p, 4s, and S 3p, the 3s orbit begin to increase and extend to the deep energy level. However, the 6s, 5p orbit of the gold surface Au also have a large change at about 6 eV when the contact distance is 8 Å, and the density of Au 6s, 5p orbit begins to increase and begins to extend to the deep energy level. This result indicates that the galvanic interaction between pyrite and gold with increasing distance leads to the enhanced electronic activity of the 3p, 4s orbit of Fe, the 3p, 3s orbit of S and the 6s, 5p orbit of Au. Combined with the calculation results of the previous part, it shows that there is electron transfer between pyrite and gold.

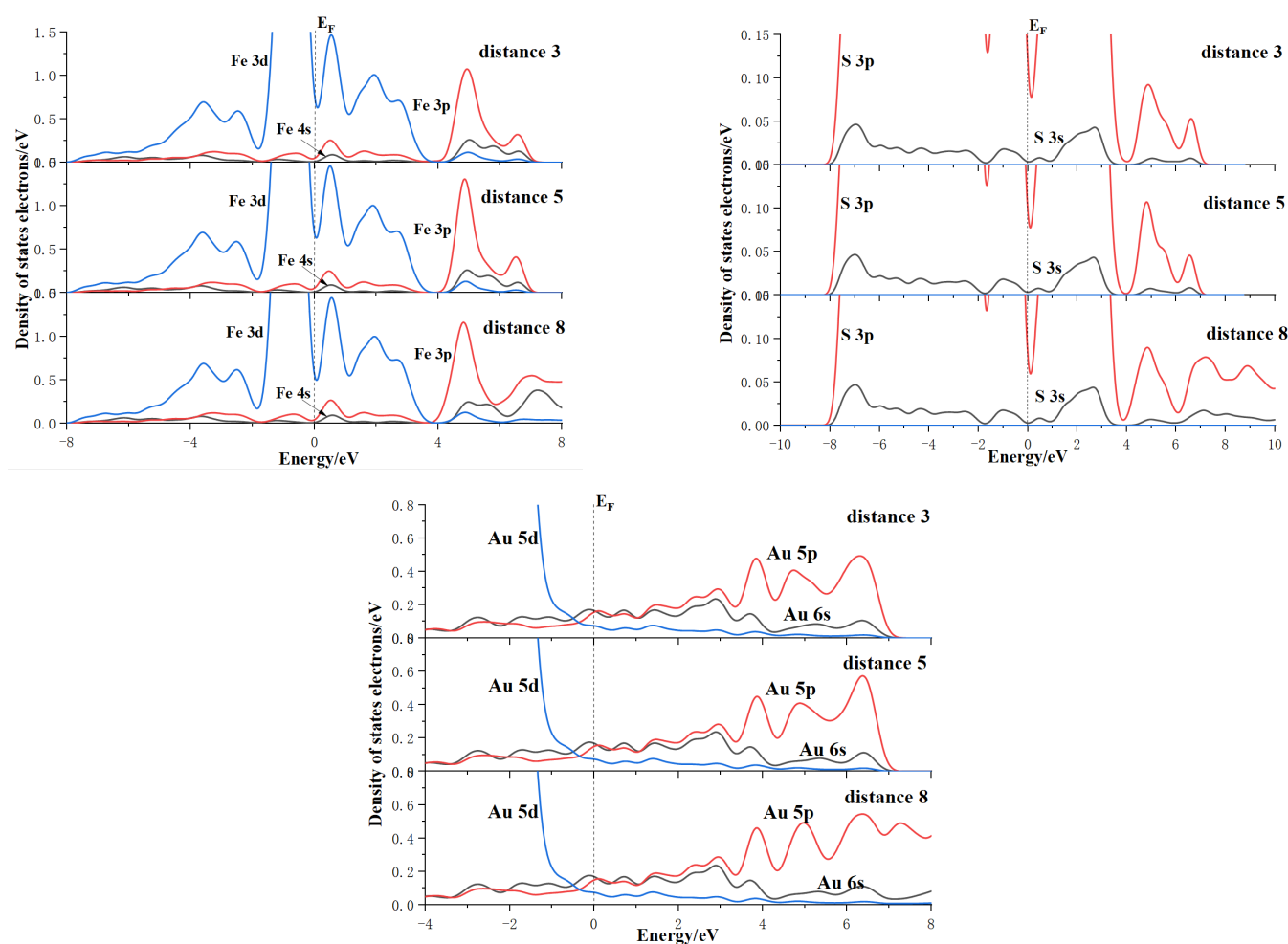


Figure 7. The density of states of Fe 3d, 3p, 4s, S 3s, 3p and Au 6s, 5p, 5d near the Fermi level (set the energy at 0 eV as the Fermi level) of pyrite and gold surface at the contact distance of 3 Å, 5 Å and 8 Å.

Figure 8 shows the density of states at the Fe, 3s, 4p and S of the gold surface, 3s, 6s, 5p and 5d at the Fermi level (set the energy to 0 eV, the Fermi level). From Figure 8, the 3d state of the poison sand surface Fe changes greatly near the Fermi level. With the increase of the contact distance, the density of states is flatter, its delocalization increases, and the density of states at the Fermi level decreases. The 4s states of As on the sand surface move towards low levels with the contact distance, and the density of states increases. This result shows that the galvanic interaction between the arsenopyrite and gold leads to the delocalization of Fe on the surface of the arsenopyrite, the electron activity of the Fe 3d orbit and the

As 4s orbit. However, the 3p orbit of S moves in the higher energy direction from 3 Å to 5 Å, and does not change at the contact distance of 8 Å. The gold surface Au moves the overall density of states towards higher energy levels as the contact distance increases from 3 Å to 5 Å, while the temporal density changes less at the contact distance of 8 Å. This indicates that the galvanic interaction between the arsenopyrite and gold on the S and gold surface at the contact distance of 8 Å. The Fe 3d orbital and As 4s orbital on the surface of arsenopyrite have a great influence on Au.

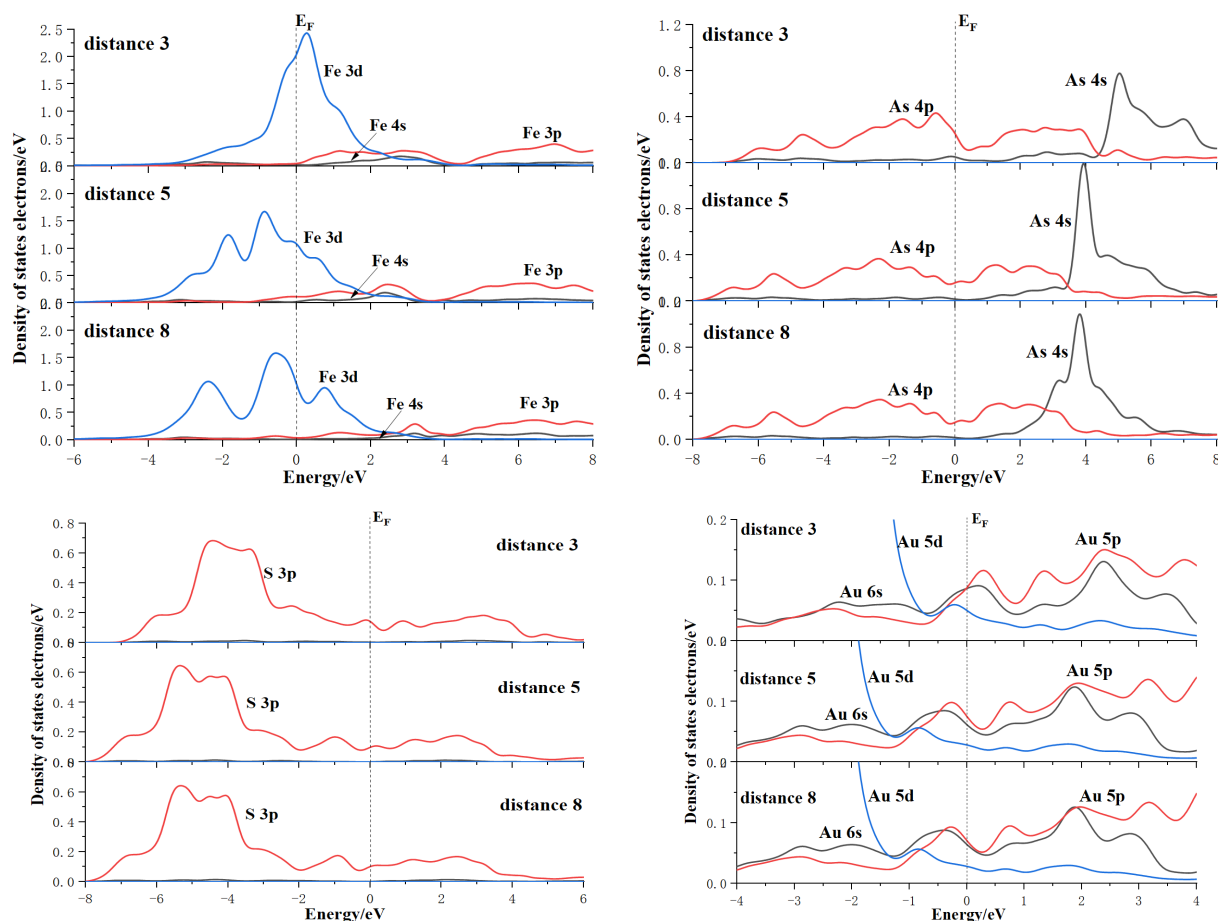


Figure 8. The density of states of Fe 3d, 3p, 4s, S 3s, 3p, As 4s, 4p and Au 6s, 5p, 5d near the Fermi level (set the energy at 0 eV as the Fermi level) of arsenopyrite and gold surface at the contact distance of 3 Å, 5 Å and 8 Å.

Figure 9 shows the density of states at the Cu 3s, 3p, 3d and S and 3p and the 6s, 5p and 5d at the gold surface near the Fermi level (set the energy at 0 eV to the Fermi level). It is known from Figure 9 that the 3s states of Cu on the chalcocite surface increase the density of states at the Fermi level as the contact distance increases. However, the density of states of S on the chalcocite surface is almost unchanged with the contact distance. However, the density of states of Au on the gold surface does not change significantly with increasing contact distance, only at about 5–7 eV. This result shows that the density of states between the chalcocite and gold is less affected by the density of states of S on the surface, and the electronic activity of the Cu 3s of the surface and the Au 5p orbit of the gold surface is enhanced.

It is found that different galvanic interaction distances have a great influence on the density of surface atoms between pyrite, arsenopyrite, and gold, but less on the density of surface atoms between chalcocite and gold pyrite. This is consistent with the calculation results of charge transfer.

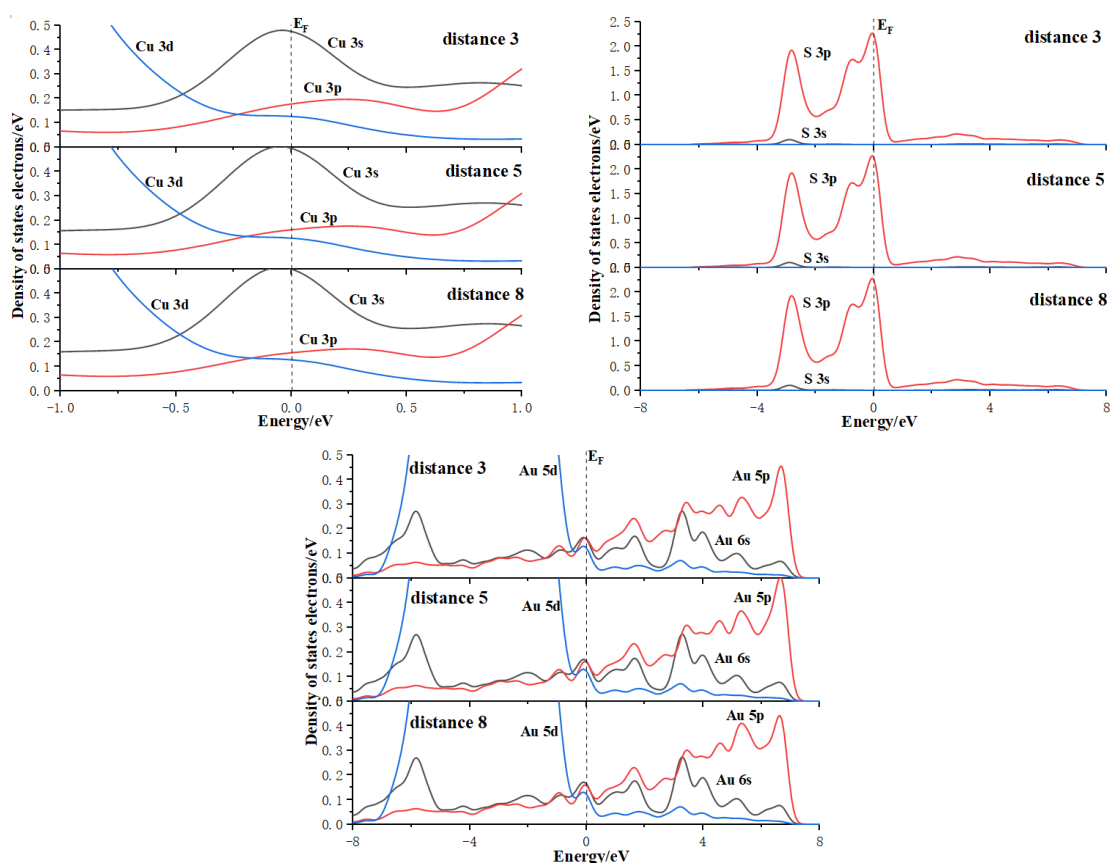


Figure 9. The density of states of Cu 3d, 3p, 4s, S 3s, 3p and Au 6s, 5p, 5d near the Fermi level (set the energy at 0 eV as the Fermi level) of pyrite and gold surface at the contact distance of 3 Å, 5 Å, and 8 Å.

4. Conclusions

The galvanic interaction of gold and associated minerals in the thiocyanate leaching of gold was analyzed objectively at the micro level by density functional theory simulation. The results show that with the increase of electrochemical distance, the number of charge transfers of pyrite also increases, and pyrite loosed electrons and inhibited the dissolution of gold. The number of charge transfers of arsenopyrite and chalcocite decreased with the increase of the distance of galvanic interaction, indicated that arsenopyrite and chalcocite obtained electrons and promoted gold dissolution. Among them, gold had the greatest influence on the gain and loss of electrons in pyrite and arsenopyrite and had the least influence on chalcocite. Therefore, in the leaching process, pyrite inhibited the leaching of gold, while arsenopyrite and chalcocite promoted the dissolution of gold. State density calculations reveal that different galvanic interaction distances had a greater effect on the state densities of surface atoms under the interaction of pyrite and arsenopyrite with gold, whereas they have a smaller effect on the state densities of surface atoms under the interaction of chalcopyrite with gold. This was also consistent with the results of charge transfer studies. The simulation results further elucidate the differences in the interaction of gold and its associated sulfide minerals and the mechanism of action.

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Data Availability Statement: The data that support the findings of this study are available from the corresponding author upon reasonable request.

Conflicts of Interest: The authors declare no conflict of interest.

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