Molecular dynamic simulations study of 2-((2-(decyloxy)ethyl)amino)lauric acid adsorption on the α-quartz (1 0 1) surface

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Abstract: Adsorption mechanism of a novel amphoteric collector 2-((2-(decyloxy)ethyl)amino)lauric acid ($CH_3(CH_2)_9CH(NH(CH_2)_3-O-(CH_2)_9CH_3)COOH$, LDEA) on the α-quartz (1 0 1) surface has been investigated through molecular dynamic (MD) simulation calculations at a molecular level. The adsorption process showed that the LDEA collector could be adsorbed onto α-quartz's (1 0 1) surface as the H atom in the polar carboxyl and amino functional group of the collector moved closer to the O atom of quartz (1 0 1) surface. The interaction energies of the collector LDEA molecule and its ionic derivative species on α-quartz surfaces in vacuum and aqueous solutions are in the order of pH 4 < pH 12 < in vacuum < pH 10 < pH 6, which demonstrating that the α-quartz (1 0 1) surface could absorb the collector LDEA in the forms of electrostatic and hydrogen bonding interactions. It also reveals that the optimal pulp pH range for LDEA adsorption on α-quartz's surface is between neutral and weak alkali environment (pH 6 - 10). The trend obtained from molecular modeling has been validated by micro-flotation studies on quartz at different pHs.

Keywords: α-quartz, molecular dynamic, 2-((2-(decyloxy)ethyl)amino)lauric acid, flotation mechanism

1. Introduction

Cationic/anionic reverse flotation has been regarded as one of the most effective technologies for separation and concentration of iron-containing minerals from fine iron-ores (Luo et al., 2016; Weng et al., 2013). This process is mainly utilizing the different surface properties between iron-containing minerals and gangue minerals. By adding appropriate reagents, the mineral surface differences become more apparent, which could lead to an enlarged flotation difference. It is essential to investigate the collector-mineral interfacial interactions so that the iron-containing minerals and gangue minerals could be separated more efficiently, and to realize the economic value of iron ore resources (Araujo et al., 2005; Hidalgo and Gutz, 2001; Xia et al., 2009).

Quartz is the common gangue mineral in iron ores. The adsorption mechanism of various collectors on quartz surface has been widely studied through traditional analysis method, such as micro-flotation tests (Lima et al., 2013; Liu et al., 2015a; Luo et al., 2018), contact angle measurements (dos Santos and Oliveira, 2007), Fourier transform infrared spectrum (FT-IR) (López-Valdivieso et al., 2000; Luo et al., 2015; Wang and Ren, 2005), X-ray photoelectron spectrum (XPS) (Wang et al., 2014; Zhu et al., 2015), surface tension (Huang et al., 2014) and atomic force microscope (AFM) (Ni and Liu, 2012) in the last several decades. Compared with the traditional methods, the new molecular simulation methods are based on first principle density theory (DFT), molecular mechanics, and semi-empirical approaches which have great potential to provide an essential sight into flotation mechanism of reagent on mineral surface, and to explore physical or chemical phenomena involved in the adsorption process at a molecule scale. Rath et al. (2014) studied the collector oleate interactions with hematite, magnetite, and

goethite by using DFT approach, and the trends obtained from quantum chemical calculation has been validated by contact angle measurements and flotation results. Zhu and co-authors studied the adsorption mechanisms of collector α-Bromolauric acid on quartz (1 0 1) surface in consideration of various factors, such as solvent water molecule, activation ion species as well as the hydrolysis and ionization equilibrium of the collector separately (Zhu et al., 2016). These studies indicate that quantum chemical simulations could be correlated to experimental techniques analyses and froth flotation behaviors. Pradip and Rai had carried out extensive work on molecular modeling to study selective flotation and selective flocculation-dispersion of minerals (Pradip and Rai, 2002, 2003; Rai et al., 2011).

From the previous studies, some significant results obtained in the vacuum system could confirm that DFT and MD simulation methods were effective ways to study molecule adsorption mechanisms. However, the depth MD simulations relating to the froth flotation which happens in a real complex aqueous environment where various factors, such as the adsorption of the solvent molecules, the phenomenon of mineral surface charge and protonation/deprotonation of collector could affect the adsorption of collector onto quartz surface have not yet been investigated. In this paper, besides the model of the interaction of collector LDEA molecule with α-quartz (1 0 1) surface in vacuum, we also attempted to fabricate several models to investigate the adsorptions of LDEA collector ionic species in the aqueous solutions, and the corresponding interaction energies were determined to be compared to micro-flotation experiment results to validate the simulation results. Moreover, the adsorption mechanisms of the novel amphoteric collector LDEA onto the α-quartz (1 0 1) surface have been studied. This study will provide the right direction towards understanding the reagent-mineral interaction in consideration of the pulp pH and developing highly selective flotation collectors for quartz separation.

2. Computational details

The MD simulation was used to fully understand the adsorption of collector molecule LDEA on α-quartz (1 0 1) surface in a vacuum environment and its ionic derivates onto α-quartz (1 0 1) surface in aqueous solutions separately. Models of α-quartz surfaces, collector LDEA, and quartz-collector complex were established on Materials Visualizer module and Amorphous Cell (AC) module. Dynamic simulations were performed under the COMPASS II (condensed-phrase optimized molecular potentials for atomistic simulation studies) force field in the Forcite module with the software package Materials Studio 8.0.

2.1. Model of the interaction of α-quartz (1 0 1) surface with LDEA molecule in vacuum

Model of the interaction of the α-quartz (1 0 1) surface with LDEA collector in vacuum was established, only in consideration of the mineral surface charge effect, that the α-quartz (1 0 1) surface is terminated mainly by naked oxygen atoms, and the LDEA is described as a neutral molecule in vacuum.

The α-quartz (1 0 1) surface with vacuum slab depth of 19.23 Å (3 layers) was cleaved from the pre-optimized quartz bulk. The face was extended to 6×5 supercell and was fitted with 60 Å to eliminate the effect of the periodic boundary firstly. Meanwhile, the geometry of the collector LDEA molecule was optimized, and the entire atoms were assigned with charges in DMol^3 module. Consequently, the LDEA molecule was implemented into the α-quartz (1 0 1) slab to construct the collector-mineral interface box 36.5 Å × 29.5 Å × 40.5 Å structure.

Then, geometry optimization was operated on the quartz-LDEA complex model to obtain the primary local minimum energy structure, which would be used as the initial configuration to explore a global minimum energy structure through MD simulation with a time step 1.0 fs in 400 ps simulation time. With one frame being collected every 5000 steps, total 81 frames were obtained (the frame before MD was included), and the lowest energy frame was selected as the best final configuration to calculate the interaction energy and measure the distances from the polar functional group to active sites of quartz surface.
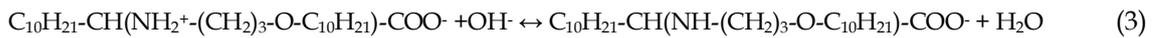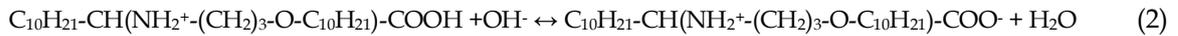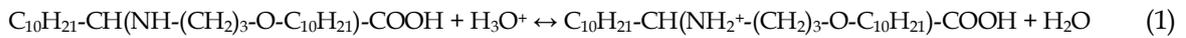
2.2. Models of the interactions of α-quartz (1 0 1) surface with LDEA ionic species in aqueous

Froth flotation takes place in the liquid phase, which means the factors such as solvent water molecules, the protonation/deprotonation of the collector molecule and α-quartz (1 0 1) surface in an aqueous

environment could also influence the adsorption of the collectors onto quartz mineral surface, which should be taken into consideration for a more accurate simulation result.

Depending on solution pHs, the α-quartz (1 0 1) surface is positively charged due to H^+ adsorption in acidic or negatively charged for adsorption of OH^- or by dissociation of H^+ in alkaline solution. The point of zero charge (PZC) of quartz is at about pH 2.0, at pH < P.Z.C., the mineral surface is positively charged, at pH > P.Z.C., the mineral surface is negatively charged (Liu et al., 2015b; Wang et al., 2016). In order to describe the surface charge effect, based on surface charge density information (Liu et al., 2015a; Zheng et al., 2001), the α-quartz (1 0 1) surface is terminated by either hydroxyl groups or naked oxygen atoms for the case of different pH conditions in MD simulation. At pH 4, the quartz surface is terminated mainly by hydroxyl groups (58 hydroxyl groups and 2 naked oxygen atom), as the surface carried a slight negative charge with a surface charge density of -30 mC·m⁻², which is consistent with the results from the previous literature (Zheng et al., 2001). At pH 6 and high pHs, the quartz surface is terminated mainly by naked oxygen atoms.

The collector LDEA when dissolved in water, gets protonated and deprotonated depending on the pH of the solution. The adsorption of LDEA on the surface of quartz can be both through molecular and ionic adsorption. The effect of pulp pH, particularly the species distribution of reagent, is essential for determining the preferred pH range for flotation. The concentration of LDEA species in aqueous solution varies with pHs and are controlled by the following reversible reactions:

$$C_{10}H_{21}\text{-}CH(NH\text{-}(CH_2)_3\text{-}O\text{-}C_{10}H_{21})\text{-}COOH + H_3O^+ \leftrightarrow C_{10}H_{21}\text{-}CH(NH_2^+\text{-}(CH_2)_3\text{-}O\text{-}C_{10}H_{21})\text{-}COOH + H_2O \qquad (1)$$

$$C_{10}H_{21}\text{-}CH(NH_2^+\text{-}(CH_2)_3\text{-}O\text{-}C_{10}H_{21})\text{-}COOH + OH^- \leftrightarrow C_{10}H_{21}\text{-}CH(NH_2^+\text{-}(CH_2)_3\text{-}O\text{-}C_{10}H_{21})\text{-}COO^- + H_2O \qquad (2)$$

$$C_{10}H_{21}\text{-}CH(NH_2^+\text{-}(CH_2)_3\text{-}O\text{-}C_{10}H_{21})\text{-}COO^- + OH^- \leftrightarrow C_{10}H_{21}\text{-}CH(NH\text{-}(CH_2)_3\text{-}O\text{-}C_{10}H_{21})\text{-}COO^- + H_2O \qquad (3)$$

Currently, for the reason that it's not realistic to obtain the constant values of K_a (association constant), K_d (disassociation constant) and K_{im} (ionomolecular complexation constant) to calculate the species concentration at a specific pH. While, the dominant species derivates could be analyzed approximately based on considering the main species of sodium oleate (NaOL) and dodecylamine (DDA) at different pHs (Pugh and Stenius, 1985; Shibata and Fuerstenau, 2003). Within the pH range, there are mainly three extant species - $C_{10}H_{21}\text{-}CH(NH_2^+\text{-}(CH_2)_3\text{-}O\text{-}C_{10}H_{21})\text{-}COOH$ ($LDEA^+$) (pH 4, and 6), $C_{10}H_{21}\text{-}CH(NH_2^+\text{-}(CH_2)_3\text{-}O\text{-}C_{10}H_{21})\text{-}COO^-$ ($LDEA^0$) (pH 10) and $C_{10}H_{21}\text{-}CH(NH\text{-}(CH_2)_3\text{-}O\text{-}C_{10}H_{21})\text{-}COO^-$ ($LDEA^-$) (pH 12). The optimal geometries of the three species of LDEA molecule were obtained and assigned with charges individually using the DMol3 module, which were used in the following Forcite calculation of the interactions between the quartz and LDEA collector.

The three species of LDEA water box - containing one collector in different ionic forms and specific number water molecules were combined with the original or hydroxylated α-quartz (1 0 1) surface supercells through Amorphous Cell module for the MD simulation. The MD simulation methods and simulation parameters settings are kept the same as in vacuum. The number of atoms in quartz and other collector species in MD simulation is summarized in Table 1. The optimized Cl^- and H^+ ions were

Table 1. Atom numbers of all species in the simulation of collector LDEA adsorption on quartz's(101) surface

Species	Atoms				
	Vacuum	pH = 4	pH = 6	pH = 10	pH = 12
LDEA	1	0	0	0	0
LDEA⁺	0	1	1	0	0
LDEA⁰	0	0	0	1	0
LDEA⁻	0	0	0	0	1
Cl⁻	0	1	1	0	0
H⁺	0	0	0	0	1
Si-O⁻	60	2	60	60	60
Si-OH	0	58	0	0	0
SiOH₂⁺	0	0	0	0	0
Bridging oxygen	480	480	480	480	480
Si	270	270	270	270	270
H₂O	0	342	342	342	342

also introduced into the models of the quartz-LDEA composites to maintain the charge balance.

2.3. The interaction energy of α-quartz (1 0 1) surface with LDEA collector calculation

The interaction energy (E_{int}) can be calculated by following Eq. 4.

$$E_{int} = E_{complex} - (E_{adsorbate} + E_{mineral}) \tag{4}$$

where $E_{complex}$ refers to the total energy of the optimized interaction configuration of quartz surface and LDEA collector, whereas $E_{adsorbate}$ and $E_{mineral}$ refer to the total energies of the quartz surface and the collector, respectively, it is worth noting that a more negative magnitude of the interaction energy indicates more favorable interactions between the collector and the mineral surface.

The convergence criteria for geometry optimation and energy calculation was set to a level of 0.001 Kcal mol^{-1}. Van der Waals force and electrostatic energy were calculated through the methods of group-based summation and Ewald summation. Cut off distance of group-based summation was 18.5 Å. QEq charge equilibration method was the only way used to calculate an atomic charge.

3.   Results and discussion

4.   The interaction of α-quartz (1 0 1) surface with LDEA molecule in vacuum

The 81 configuration adsorption energy values of the collector LDEA molecule on the α-quartz (1 0 1) surface during the 400ps simulation time were shown in Fig. 1.
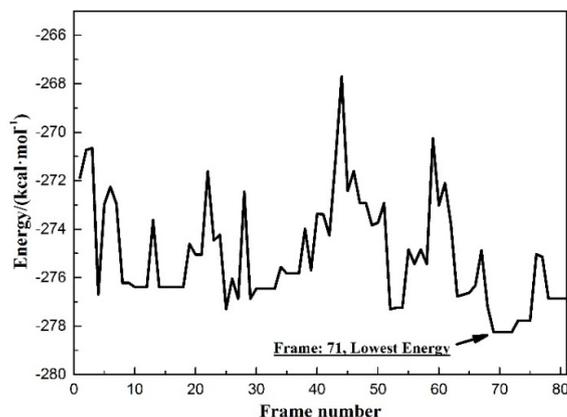

Fig. 1. Adsorption energy values of the 81geometries of collector LDEA on α-quartz (101) surface during the simulation time 400 ps
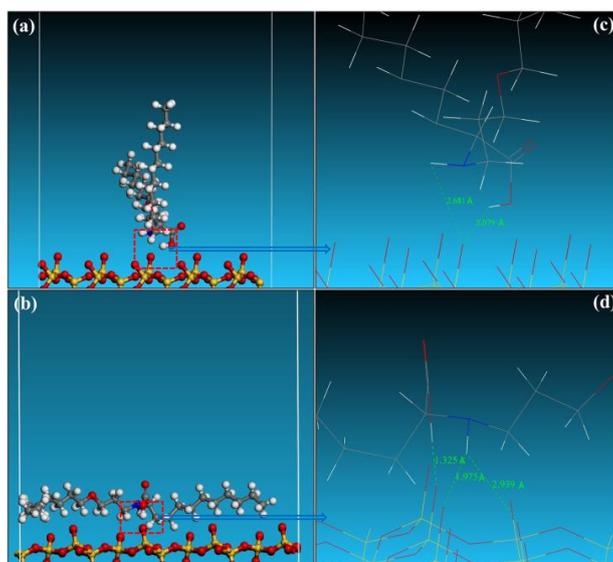

Fig. 2 The initial (a) and the collector LDEA interaction with α-quartz (101) surface lowest energy equilibrium configurations (b) in vacuum. (O = red, Si = yellow, N = blue, C = gray, H = white)

As shown in Fig. 1, the seventy-first geometry is the lowest energy configuration in 400 ps simulation time, which was a relatively global stable structure (Fig. 2b). Compared with the initial adsorption configuration (Fig. 2a), it can be found that alkyl chain of collector LDEA molecule lying on α-quartz (1 0 1) surface (Fig. 2b). As we know, the hydrophobicity of mineral is achieved through the reduction of the exposed part of mineral surface to aqueous phase by the covering of the collector and the blocking layer of the alkyl chain. To some extent, the more coverage of the collector, the better hydrophobicity will be obtained. The adsorption process of LDEA molecule onto α-quartz's (1 0 1) surface illustrates that the LDEA collector could adsorb on quartz's surface as the H atom of collector moved closer to the active site O atom of α-quartz (1 0 1) surface. It can be seen that the -OH (in -COOH group) adsorbed on quartz surface approximately perpendicular, while an angle of the incline was founded between the N-H bond of the collector and quartz surface. It indicates the formations of two types of hydrogen bonds presented by the green dotted lines between the carboxyl group and amino group and the Si-O active sites. The relative O-H···O and N-H···O are characterized by an H-bond length of 1.325 Å and 1.975 Å. The calculated interaction energy between collector molecule and α-quartz (1 0 1) surface in vacuum is -254.14 kcal·mol^{-1}, which illustrate a strong hydrogen bonding adsorption ability of LDEA on the quartz surface.

4.1. The interactions of α-quartz (1 0 1) surface with LDEA ionic species in solution

The equilibrium configurations of collector LDEA ionic derivative species (LDEA$^+$, LDEA^0, and LDEA$^-$) on α-quartz (1 0 1) surface under different pHs are shown in Fig.3. The distances from the O and H atoms of the polar group (-COOH and -NH-) of the collector LDEA to the H and O atoms of α-quartz (1 0 1) surface are shown in Fig.4. The relationships between the interaction energies of collector LDEA onto α-quartz's (1 0 1) surface and quartz single mineral recoveries are shown in Table 2.
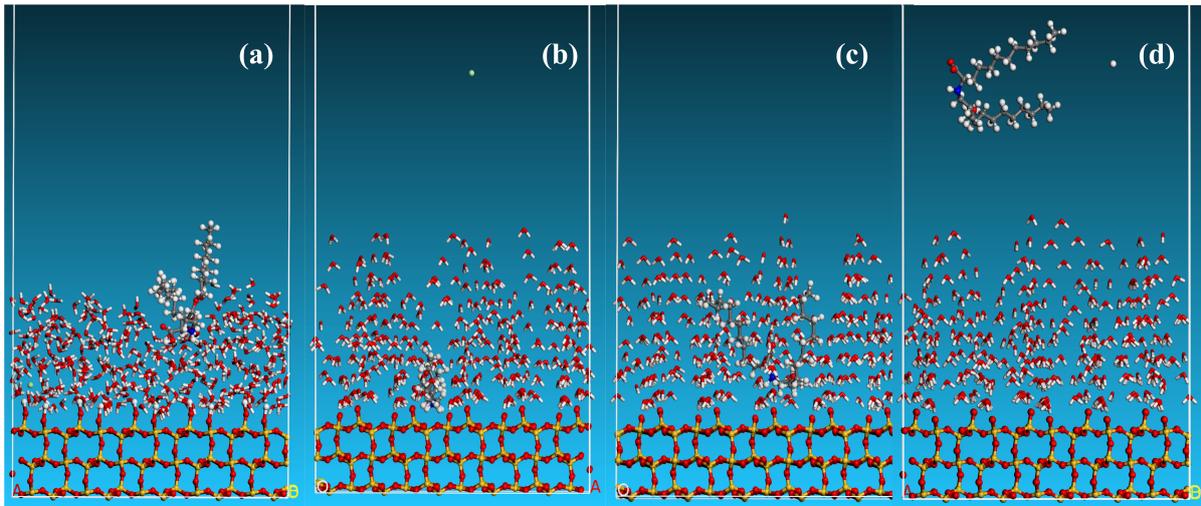

Fig. 3 Equilibrium configurations of LDEA species on α-quartz (101) surface under pH 4 (a), pH 6 (b), pH 10 (c) and pH 12 (d) in solution. (O = red, Si = yellow, N = blue, C = gray, H = white, Cl = green)

Table 2 The relationship between adsorption energies of collector LDEA on quartz's (101) surface and quartz single mineral recoveries

pH	$E_{collector}$(kcal·mol^{-1})	$E_{mineral}$(kcal·mol^{-1})	E_{total}(kcal·mol^{-1})	E_{int} (kcal·mol^{-1})	Recovery (%)
4	8.70	22181.55	22198.56	8.31	76.56
6	57.74	39993.72	38683.48	-1367.98	94.15
10	85.10	39993.72	39626.61	-452.21	94.55
12	49.19	39993.72	40098.60	55.69	2.97

As shown in Fig. 3, the optimization configurations of collector LDEA in aqueous solution is different from that in vacuum. Under pH 4, the reduction impact of the collector to water molecules is weak. The distances between from the polar function group to hydroxylation quartz surface are more than 6.9 Å (Fig. 4a), and relatively energy is 8.31 kcal·mol^{-1}, which illustrated that a strong acid condition is not favorable for the flotation recovery of the quartz. With raising pH from 4 to 6, the collector represented a relative strong repulsion force to water molecules with lying on the quartz surface, and the distances are about 1.5 Å which means strong adsorption of collector LDEA on quartz surface and the hydrophobicity could be enhanced much.
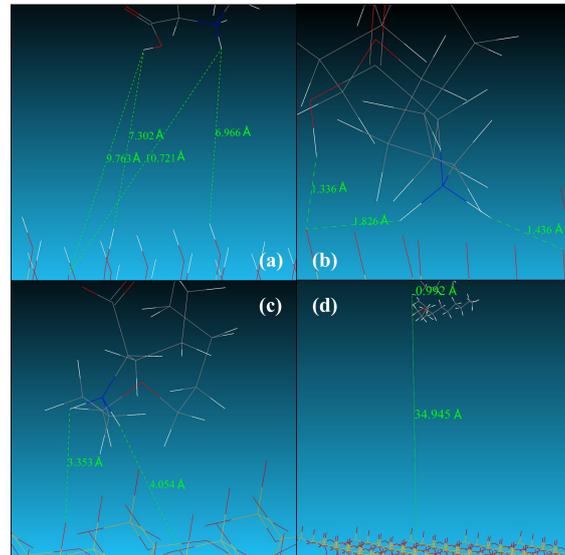

Fig. 4 Distances from the O and H atoms of -COOH and -NH- polar group of the collector LDEA to the H and O atoms of α-quartz (1 0 1) surface under pH 4 (a), pH 6 (b), pH 10 (c) and pH 12 (d) in solution. (O = red, Si = yellow, N = blue, C = gray, H = white, Cl = green)

Compared the configurations under pH 6 and 10, it can be easily found that the decreasing of reduction impact of the collector to water molecules and the distances between from functional group to active sites on quartz surface (Fig. 4b-c), and relatively interaction energies decreased from -1367.98 kcal·mol^{-1} to -452.21 kcal·mol^{-1}, meaning a neutral to weak alkali (pH 6 - 10) environment would be beneficial for quartz mineral flotation. Moreover, the results suggest that ionic electrostatic adsorption is much stronger than molecular hydrogen bonding adsorption (Fig. 2). With increasing pH to 12, the collector was going away from the quartz surface, and the calculated interaction energy was 55.69 kcal·mol^{-1}, which illustrates that the strong alkaline is not detrimental for the flotation of the quartz. Trends obtained from the molecular dynamic simulation corresponding well with the miro-flotation results (Table 2)(Luo et al., 2018).

5.   Conclusions

The MD simulations of the interactions of collector LDEA with quartz surface have been proven to be an effective way to study the adsorption mechanisms and processes of the collector LDEA onto the α-quartz (1 0 1) surface. The collector LDEA could be adsorbed on the surface of the quartz in the forms of electrostatic and hydrogen bonding interactions. The adsorptions can be affected by pHs, where a neutral to weak alkali environment could enhance the interaction forces between the collector and quartz surface, which are in good accordance with the interaction energies and the flotation results.

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