Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Adsorption of Poly Acrylic Acid onto the Surface of Calcite: an Experimental and Simulation Study.

Supplementary Information

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Here the potential parameters for the poly acrylic acid polymer are given. Table 1 gives an overview of the atomic symbols used throughout the work and the atomic charges. Table 2 gives an overview of the bonds and angles used within this work, with the functional forms for the bonds and angles detailed in Equations 1 and 2 respectively. The dihedral angles of the polymer are given in Table 3 and are of the form in Equation 3. The intermolecular terms between the polymer and the mineral/water are of the AB 12-6 and Buckingham functional forms (Equations 4 & 5) and are presented in Tables 4 & 5.

Table 1: Atom types and atomic charges used in this work

PAA			**$CaCO_3$ & water**		
Symbol	Charge (au)	PAA atom type	Symbol	Charge (au)	Other atom type
C1	-0.0737	terminal carbon	CA	2.0000	calcium ion
C1	-0.0409	CH2 carbon	C	1.1233	carbon of carbonate ion
C1	-0.1477	CHCOO- backbone carbon	O	-1.0411	oxygen of carbonate ion
CC	0.9150	carboxyl carbon	OW	-0.8340	oxygen of water
OC	-0.9130	carbonyl oxygen	HW	0.4170	hydrogen of water
H1	0.0171	Hydrogen of CT carbon			
H1	0.0262	Hydrogen of CH2 carbon			
H1	0.0528	Hydrogen of CHCOO- carbon			

$$U(r) = \frac{1}{2}k(r - r_0)^2 \tag{1}$$

$$U(\theta) = \frac{k}{2}(\theta - \theta_0)^2 \tag{2}$$

$$U(\phi) = A[1 + cos(m\phi - \delta)] \tag{3}$$

$$U(r) = (\frac{A}{r^{12}}) - (\frac{B}{r^6}) \tag{4}$$

$$U(r) = Aexp(-\frac{r}{\rho}) - \frac{C}{r^6} \tag{5}$$

Table 2: PAA intramolecular terms - bonds and angles

Bonds			**Angles**		
Bond	k (kJ mol^{-1} Å^{-2})	r_0 (Å)	Angle	k (kJ mol^{-1} rad^{-2})	θ_0 (deg)
C1 C1	2538.0381	1.5350	C1 C1 H1	388.2838	110.056
C1 CC	2749.0528	1.5080	C1 CC H1	395.2339	109.680
CC OC	5426.0928	1.2140	OC CC OC	654.5643	130.380
CC H1	2824.4152	1.0920	H1 C1 H1	330.1710	108.350
			OC CC C1	569.6560	123.110
			CC C1 C1	534.1519	110.530
			C1 C1 C1	529.2952	110.630

Table 3: PAA intramolecular terms - dihedrals

Dihedral	A (kJ mol^{-1})	m	δ_a (deg)	Dihedral	A (kJ mol^{-1})	m	δ (deg)
C1 C1 C1 H1	0.6698	3	0	H1 C1 C1 H1	0.6280	3	0
CC C1 C1 H1	0.6512	3	0	C1 C1 C1 C1	0.7536	3	0
H1 C1 CC OC	3.3494	1	0	C1 C1 CC OC	0.8373	3	180
H1 C1 CC OC	0.3349	3	180	C1 C1 C1 CC	0.6512	3	0

Table 4: Intermolecular terms - 12-6

	A (kJ mol^{-1} Å^{-12})	B (kJ mol^{-1} Å^{-6})		A (kJ mol^{-1} Å^{-12})	B (kJ mol^{-1} Å^{-6})
C1 C1	4367168.3069	2828.6533	H1 H1	31468.3113	90.9615
C1 CC	3872045.8800	2507.9582	C1 OW	3290574.2908	2664.06319
C1 O	2712383.7593	2623.9516	CC OW	2917509.4066	2362.0282
C1 H1	406834.7544	531.3850	OC OW	1979952.4366	2432.6108
CC CC	3433057.3544	2223.6214	H1 OW	289587.4783	486.5014
CC OC	2404870.5299	2326.4642	C1 O	55486.4674	183.3127
CC H1	360710.3555	471.1399	CC O	49195.7562	162.5298
OC OC	1590466.5073	2365.0646	OC O	26516.9115	149.1753
OC H1	227871.2130	468.1074	H1 O	3217.3484	27.1727

Table 5: Intermolecular terms - Buckingham

	A (kJ mol^{-1})	ρ (Å)	C (kJ mol^{-1} Å^{-6})
CA OC	104684.0984	0.2970	0.0
OC OW	48241.6996	0.2300	0.0