Non Bonding Potentials $\frac{qq}{r} + \left(E_0 \left[\left(\frac{R_0}{r}\right)^{12} - 2\left(\frac{R_0}{r}\right)^{6}\right]\right)$				
Description	Symbol	q/au	R_0/Å	E_0/eV
Sp3 Carbon	CT	-0.3660	3.816	0.00475
Oxygen in Alcohol Group	OH	-0.5783	3.442	0.00913
Hydrogen in —CH_3	HC	0.1323	2.974	0.00068
Hydrogen in —CH_2—	H1	0.0956	2.774	0.00068
Hydrogen in Alcohol Group	HO	0.4188	—	—

Harmonic Bonding Potentials $(k(r - r_0)^2)$		
Atom Pair	k/eV	r_0/Å
CT—CT	13.4487	1.52
CT—OH	13.8825	1.41
CT—HC	14.7502	1.09
CT—H1	14.7501	1.09
OH—HO	23.9907	0.96

Three Body Potentials $(k(\theta - \theta_0)^2)$		
Atoms	k/eV	$\theta_0/^\circ$
CT—CT—OH	2.1691	109.5
CT—CT—H1	2.1691	109.5
CT—CT—HC	2.1691	109.5
CT—OH—HO	2.3861	108.5
OH—CT—H1	2.1691	109.5
HC—CT—HC	1.5184	109.5
H1—CT—H1	1.5184	109.5

Dihedral Potentials $A[1 + \cos(m\phi - \delta)]$			
Atoms	A/eV	$\delta/^\circ$	m
HC—CT—CT—OH	0.0607	0.000	3.000
HC—CT—CT—H1	0.0607	0.000	3.000
CT—CT—OH—HO	0.0217	0.000	3.000
H1—CT—OH—HO	0.0217	0.000	3.000

Table 1: Potential parameters used for Ethanol: non-bonding potentials are combined using the mixing rules $R_{ij} = 0.5(R_i + R_j)$ and $E_{ij} = \sqrt{E_i E_j}$

.

Non Bonding Potentials $\frac{qq}{r} + \left(E_0 \left[\left(\frac{R_0}{r}\right)^{12} - 2\left(\frac{R_0}{r}\right)^{6}\right]\right)$				
Description	Symbol	q/au	R_0/Å	E_0/eV
Oxygen in Water	OW	-0.834	3.537	0.00659
Hydrogen in Water	HW	0.417	—	—-

Harmonic Bonding Potentials $(k(r - r_0)^2)$		
Atom Pair	k/eVÅ^{-2}	r_0/Å
OW—HW	23.991	0.9572

Three Body Potentials $(k(\theta - \theta_0)^2)$		
Atoms	k/eV	θ_0/°
HW—OW—HW	4.3383	104.5

Table 2: Potential parameters used for Water

Atomic Species and Charges		
Description	Symbol	q/au
Calcium Ion	CA	2.0
C in Carbonate group	C	1.135
O in Carbonate group	O	-1.04A

Ion Pair Potentials $A\exp\left(\frac{-r}{\rho}\right) - \frac{C}{r^6}$			
Ion Pair	A/eV ρ/Å	C/eVÅ^6	
CA—O	1550.0	0.297	0.0
O—O	16372.0	0.213	3.47

Morse Bonding Potential $E_0\left[\{1-\exp\left(-k\left(r-r_0\right)\right)\}^2-1\right]$			
Ion Pair	E_0/eV	r_0/Å	k//AA^{-1}
C—O	4.71	1.18	3.80

Three Body Potentials $(k(\theta-\theta_0)^2)$		
Atoms	k/eV	$\theta_0/^\circ$
O—C—O	1.69000	120.0

Dihedral Potentials $A[1+\cos(m\phi-\delta)]$			
Atoms	A/eV	$\delta/^\circ$	m
C—O—O—O	0.1129	180.0	2.000

Table 3: Potential parameters used for modelling $CaCO_3$

BUCKINGHAM POTENTIALS: $A\exp\left(\frac{-r}{rho}\right) - \frac{C}{r^6}$			
Ion Pair	A/eV ρ/Å	C/eVÅ^6	
CA—OW	1186.6	0.297	0.0
CA—OH	1000.0	0.297	0.0

LENNARD JONES POTENTIALS: $\frac{A}{r^m} - \frac{B}{r^n}$				
Ion Pair	m	n	A/eVÅ^m	B/eVÅ^n
O—OW	9	6	2542.156	38.419
O—CT	12	6	19942.854	11.198
O—OH	12	6	15357.080	11.571
O—HC	12	6	1923.243	2.140
O—H1	12	6	1357.050	1.798
C—CT	12	6	45251.855	29.310
C—OH	12	6	34339.488	30.068
C—HC	12	6	4215.553	5.506
C—H1	12	6	2944.708	4.602
OW—CT	12	6	34094.195	27.621
OW—OH	12	6	25271.035	28.004
OW—HC	12	6	3001.113	5.044
OW—H1	12	6	2063.851	4.183

Table 4: Cross terms used for modelling interactions between Water / Ethanol, Water / $CaCO_3$ and Ethanol / $CaCO_3$.