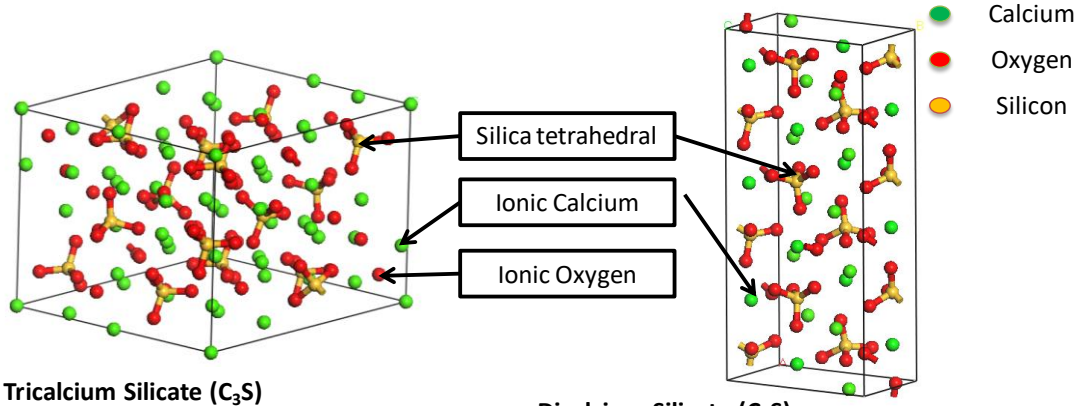
Supplementary Information

Unit Cells

The unit cells of Tricalcium and Dicalcium Silicate



Tricalcium Silicate (C_3S)
[Golovastikov,1975]

$C_3S \rightarrow (CaO)_3 (SiO_2)$

$3Ca^{x+} + SiO_4^{y-} + O^{z-}$

Dicalcium Silicate (C_2S)
[Nevski,1982]

$C_2S \rightarrow (CaO)_2(SiO_2)$

$2Ca^{x+} + SiO_4^{y-}$

Lattice Parameters

	a	b	c	α	β	γ
C_3S	11.670 Å	14.240 Å	13.720 Å	105.50^0	94.33^0	90.00^0
C_2S	20.871 Å	9.496 Å	5.600 Å	90.00^0	90.00^0	90.00^0

Potential Function

$$E_{pot} = \sum_{ij\ bonded} K_{r,ij}(r_{ij} - r_{0,ij})^2 + \sum_{ijk\ bonded} K_{\theta,ijk}(\theta_{ijk} - \theta_{0,ijk})^2 + \frac{1}{4\pi\varepsilon_0\varepsilon_r} \sum_{ij\ nonbonded} \frac{q_i q_j}{r_{ij}} + \sum_{ij\ nonbonded} \varepsilon_{0,ij} \left[\left(\frac{\sigma_{0,ij}}{\sigma_{ij}} \right)^{12} - 2 \left(\frac{\sigma_{0,ij}}{\sigma_{ij}} \right)^{6} \right]$$

Bonded Interactions

Bonds	**r_0 (Å)**	**K_r (kcal/mol- Å^2)**
Si-O	1.6800	250
O-H	0.9572	450

Angles	**θ_0 (rad)**	**K_θ (kcal/mol- rad^2)**
O-Si-O	109.50	160
H-O-H	104.52	55

Non-bonded Interactions

Element	**Charge**	**$\sigma_{0,ii}$ (Å)**	**$\varepsilon_{0,ii}$ (kcal/mol)**
Ca	1.50	3.3500	0.2800
Si	1.00	4.5000	0.4700
O_{bonded}	-1.00	3.1500	0.0800
$O_{nonbonded}$	-1.50	3.5000	0.0800
O_{water}	-0.82	3.5367	0.1521
H_{water}	0.41	0.4490	0.0460