Submitted to: *Chemistry of Materials*, July 25, 2001

Revised version

Supporting information

to the paper of A. G. Kalinichev and R. J. Kirkpatrick

"Molecular dynamics modeling of chloride binding to the surfaces of Ca hydroxide, hydrated Ca-aluminate and Ca-silicate phases"

Table 1s. Force filed parameters of the simulation model. [a]

	σ_{ii} / Å	ε_{ii} / kJ/mol	q_i / e
Oxide / hydroxide structure			
Ca	5.56	2.10×10^{-5}	1.05
Al	4.27	5.56×10^{-6}	1.575
O (portlandite)	3.166	0.650	–0.95
O (Friedel's salt)	3.166	0.650	–0.87083
O (ettringite)	3.166	0.650	–0.8675
O1 (tobermorite)	3.166	0.650	–1.1305
O2 (tobermorite)	3.166	0.650	–1.0808
H (hydroxide)	—	—	0.425
Interlayer and aqueous species			
O (water) [b]	3.166	0.650	–0.82
H (water) [b]	—	—	+0.41
Cl^- [c]	4.401	0.418	–1.0
Na^+ [c]	2.584	0.418	+1.0
K^+ [c]	3.332	0.418	+1.0
Cs^+ [c]	3.884	0.418	+1.0
S (SO_4) [d]	3.55	1.046	+2.0
O (SO_4) [d]	3.15	0.837	–1.0

[a] Cygan, R. T.; Liang, J.; Kalinichev, A. G. *J. Phys. Chem. B* **2002**, submitted.

[b] Berendsen, H.J.C. et al. *In: Intermolecular Forces*; Pullman, B., ed., Riedel, Dordrecht, **1981**, p.331.

[c] Dang, L. X. *J. Am. Chem. Soc.* **1995**, *117*, 6954.

[d] Cannon, W. R.; Pettitt, B. M.; McCammon J. A. *J. Phys. Chem.* **1994**, *98*, 6225.

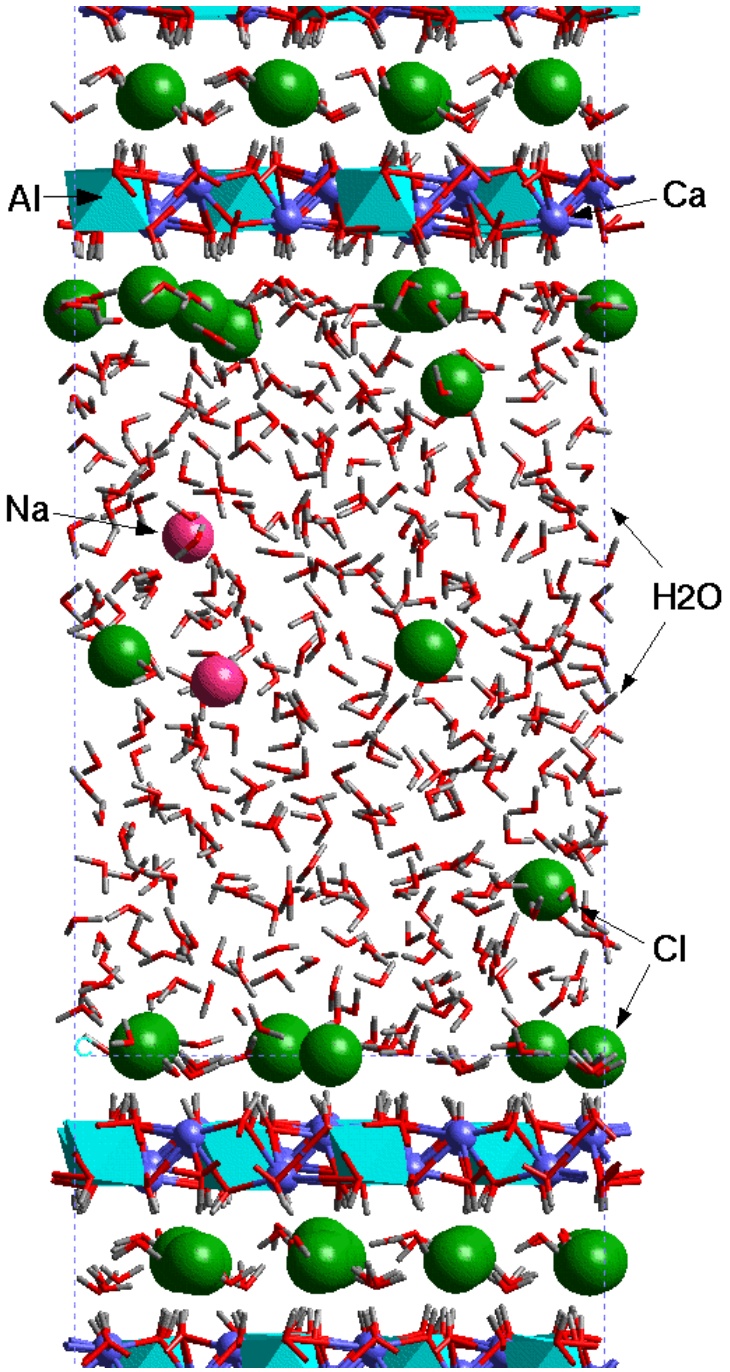

Fig. 1s. A simulation snapshot of the Friedel's salt, $[Ca_2Al(OH)_6]Cl{\cdot}2H_2O$, interface with 0.28*m* NaCl aqueous solution. Dark blue balls – Ca; light blue octahedra – Al; red cylinders – O; gray cylinders – H; green balls – Cl ions; pink balls – Na ions. Only parts of the solid layer are shown above and below the solution layer.

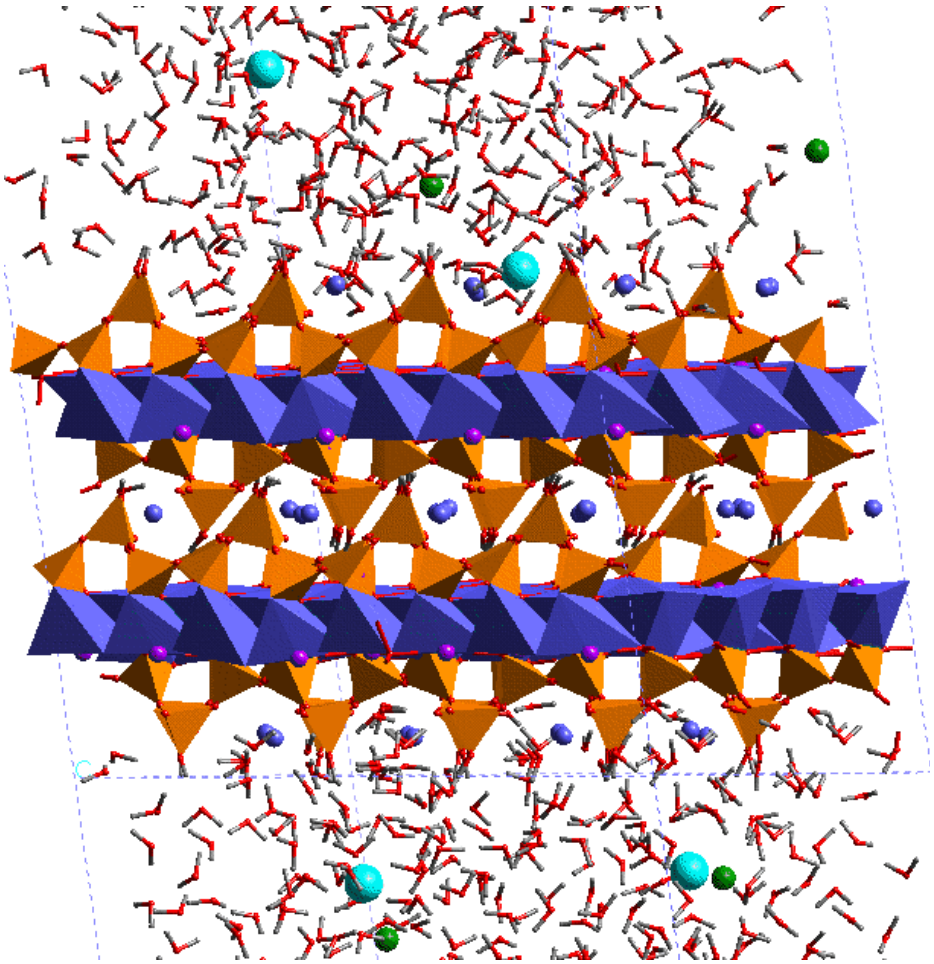

Fig. 2s. A simulation snapshot of the tobermorite, $Ca_5Si_6O_{16}(OH)_2$, interface with 0.25*m* KCl aqueous solution. Dark blue balls and octahedra – Ca atoms in two different structural positions within the "tobermorite 9 Å" structure (Merlino et al., 1999); orange tetrahedra – Si; red cylinders – O; gray cylinders – H; green balls – Cl ions; light blue balls – K ions. Only parts of the solution layer close to the interface are shown above and below the solid layer.

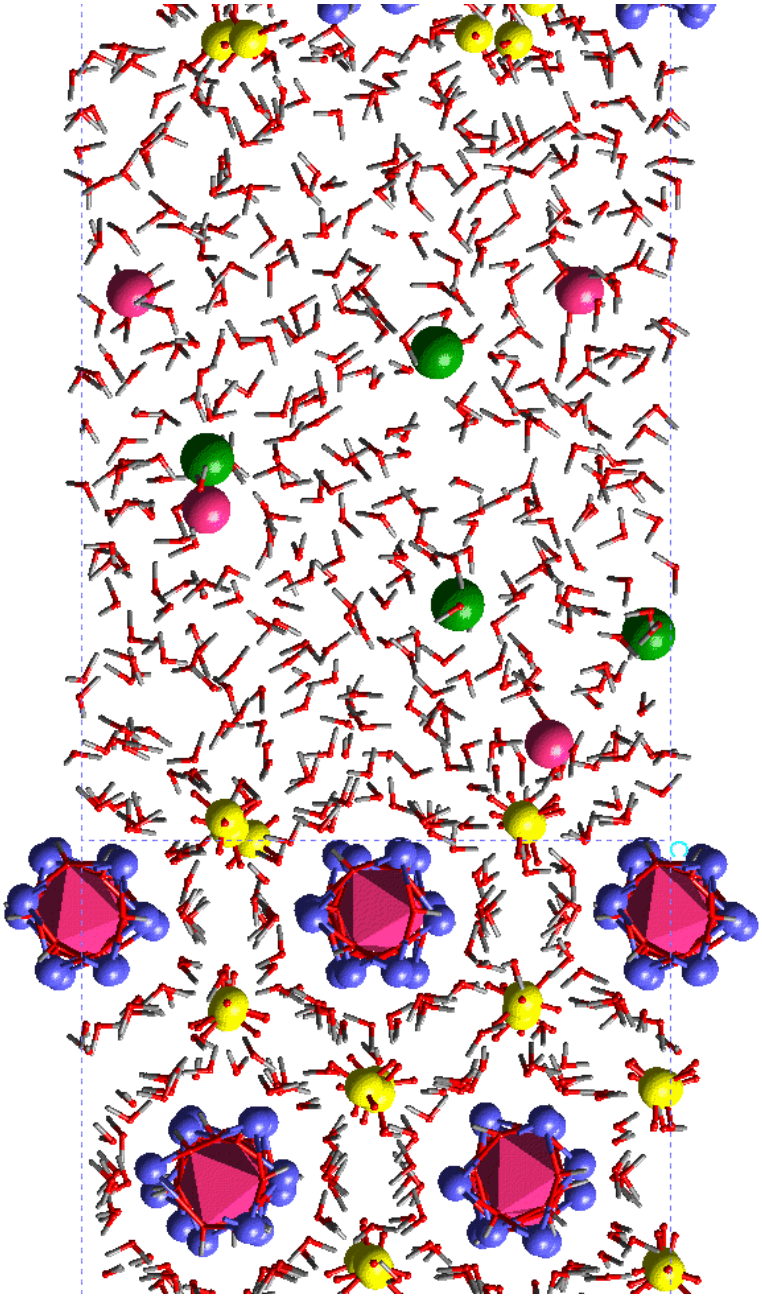

Fig. 3s. A simulation snapshot of the ettringite, $Ca_6[Al(OH)_6]_2[SO_4]_3 \cdot 26H_2O$, interface with 0.4*m* NaCl aqueous solution. Dark blue balls – Ca; pink octahedra – Al; red cylinders – O; gray cylinders – H; green balls – Cl ions; pink balls – Na ions; yellow balls – S of sulfate ions. Only parts of the solid layer are shown above and below the solution layer.