SUPPORTING INFORMATION

Cs-137 immobilization in C-S-H gel nanopores

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Topological analysis

As a consequence of the chemical and structural relaxation done with the reactive force field ReaxFF[1] the local environment of the atoms changes. Thus, it is necessary to carry out a topological analysis, leading to 1 type of silicon, 2 types of calciums, 6 types of oxygens and 3 types of hydrogens (see Figure S1). Ca1 and Ca2 correspond to the intralaminar and interlaminar Ca ions of C-S-H. O1 and H1 are the oxygen and hydrogen atoms of silanol groups, O2 corresponds to the bridging oxygen atoms of silicate chains, while O3 and O4 are terminal oxygen atoms from the inner and outer faces of the silicate chains. O5 and H5 are the oxygen and hydrogen atoms of hydroxyl groups, whereas O6 and H6 are the oxygen and hydroxyl atoms of water molecules. Moreover, Cs corresponds to the cesium cations under study.

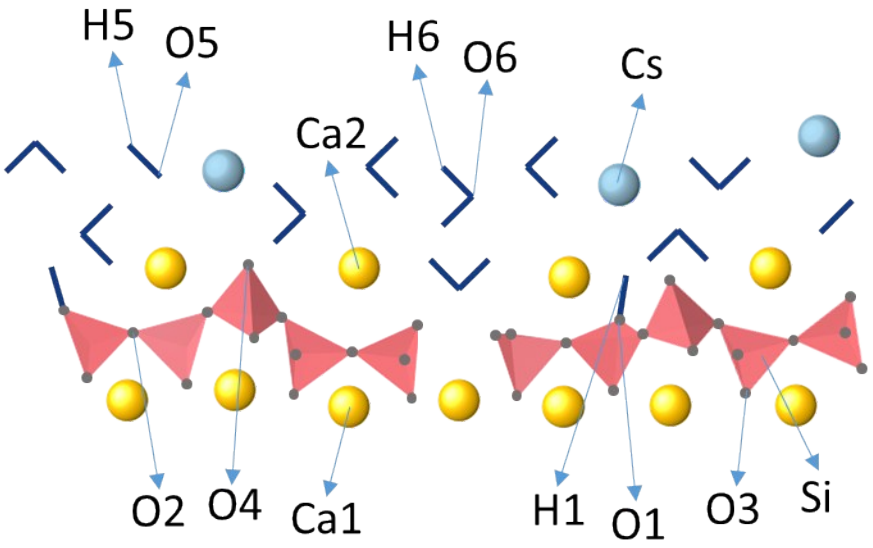

Figure S1. Schematic representation of a C-S-H layer with the label of the different atom types after the topological analysis.

Partial charges

The partial charges employed in the simulation of the C-S-H systems are given in Table S1.

Table S1. Partial charge of species provided by CSHFF[2], ClayFF[3] and flexible SCP water model[4].

Atom type	Charge
Ca1	+1.430
Ca2	+2.000
Cs	+1.000
H1	+0.290
H5	+0.425
H6	+0.410
O1	-1.000
O2	-1.140
O3	-1.07016
O4	-1.07016
O5	-0.950
O6	-0.410
Si	+1.720

Potential parameters

The potential parameters employed in the simulation of the C-S-H systems are given in Table S2.

Table S2. Potential parameters for the species in our samples.

$spec_i$	$spec_j$	ε (kCal/mol)	σ (Å)
Ca1	**Ca1**	0.0000050298	5.567
Ca2	**Ca2**	0.1000	2.872
Cs	**Cs**	0.1000	3.831
H1	**H1**	0.0000	0.000
H5	**H5**	0.0000	0.000
H6	**H6**	0.0000	0.000
O1	**O1**	0.0618	3.448
O2	**O2**	0.0618	3.448
O3	**O3**	1.2430	2.735
O4	**O4**	1.2430	2.735
O5	**O5**	0.1554	3.166
O6	**O6**	0.1554	3.166
Si	**Si**	0.0000018405	3.302

Bond stretch and angle bend parameters

The potential parameters employed in the simulation of the C-S-H systems are given in Table S3.

Table S3. Bond stretch and angle bend parameters.

$spec_i$	$spec_j$	k_1 (kCal/mol Å²)	r_0 (Å)
H1	**O1**	554.135	1.000
H5	**O5**	554.135	1.000
H6	**O6**	554.135	1.000

$spec_i$	$spec_j$	$spec_k$	k_2 (kCal/mol θ²)	θ_0 (˚)
H6	**O6**	**H6**	45.770	109.47

Bibliography

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