Electronic Supplementary Information

Atomic-scale models of early-stage alkali depletion and SiO_2-rich gel formation in bioactive glasses

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Table S1: Potential parameters

Core-shell harmonic potential: $V(r) = 0.5kr^2$

interaction	k (eV Å^{-2})
$O_C^{0.8482}$ - $O_S^{-2.8482}$	74.92
$Oh_C^{0.9}$ - $Oh_S^{-2.3}$	74.92

Buckingham potential: $V(r) = Ae^{-r/\rho} - Cr^{-6}$

interaction	A (eV)	ρ (Å)	C (eV Å^6)
O_S-O_S	22764.3	0.149	27.88
Si-O_S	1283.91	0.32052	10.66158
Si-Oh_S	983.556	0.32052	10.66158
P-O_s	1120.0913	0.334772	0
P-Oh_S	814.2	0.334772	0
Na-O_S	56465.3453	0.193931	0
Na-Oh_S	47095.911	0.193931	0
Ca-O_S	2152.3566	0.309227	0.09944
Ca-Oh_S	1222.715	0.309227	0.09944
Oh_S-O_S	22764.3	0.149	13.94
Oh_S-Oh_S	22764.3	0.149	6.97
O_S-H	311.97	0.25	0
Oh_S-H	311.97	0.25	0

Morse potential: $V(r) = D[1-\exp(-\beta(r-r_0)]^2$

interaction	D(eV)	β (Å^{-1})	r_0 (Å)
O_S-H	7.0525	3.17490	0.9485

Three-body potential: $V^{OTO}(\theta_{ijk}) = 0.5k(\theta_{ijk} - \theta_0)^2\exp[-(r_{ij}^8+r_{ik}^8)/\rho^8]$

interaction	k (eV rad^{-2})	θ_0 (deg)	ρ (Å)
O-Si-O (O=O_S, Oh_S)	6.150	109.47	1.95
O-P-O (O=O_S, Oh_S)	3.075	109.47	1.95