Surface structure and stability of partially hydroxylated silica surfaces

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Table S1: Pair distribution functions (PDF) and bond angle distributions (BAD) for silica surfaces simulated using ClayFF classical MD forcefield. Location of peak height is reported along with the full-width-at-half-max as the variation.

		100%	80%	60%	40%	20%	0%
ReaxFF	Si-Si (Å)	3.12±0.17	3.13±0.17	3.13±0.17	3.14±0.17	3.13±0.17	3.13±0.17
	O-O (Å)	2.54±0.31	2.54±0.24	2.54±0.35	2.52±0.20	2.53±0.24	2.54±0.27
	O-H (Å)	0.98±0.03	0.98±0.03	0.98±0.03	0.98±0.03	0.98±0.04	-
	O-Si-O (°)	108±17	108±17	107±17	107±17	107±16	108±16
	Si-O-H (°)	124±5	125±5	125±5	125±5	124±5	-
ClayFF	Si-Si (Å)	3.11±0.23	3.11±0.24	3.10±0.24	3.10±0.24	3.09±0.22	3.10±0.21
	O-O (Å)	2.57±0.15	2.56±0.17	2.56±0.17	2.56±0.17	2.56±0.17	2.56±0.17
	O-H (Å)	1.03±0.02	1.03±0.03	1.03±0.03	1.03±0.03	1.02±0.03	-
	O-Si-O (°)	109±13	108±13	108±13	108±13	108±13	108±14
	Si-O-H (°)	119±6	118±10	119±12	119±11	119±11	-

Table S2: Changing Q_n speciation of the silica surface structure with hydroxylation (0-100% hydroxyl coverage). Q_1 concentrations are less than 0.2 for all simulation methods and hydroxylation levels.

		100%	80%	60%	40%	20%	0%
ReaxFF	Q_5	5.01±0.44	5.51±0.48	5.77±0.86	5.94±0.43	5.34±21	4.58±0.21
	Q_4	66.81±3.56	66.84±3.13	66.41±3.79	66.75±3.03	66.67±3.27	66.41±3.60
	Q_3	24.11±2.69	23.41±2.53	23.58±2.28	23.49±2.22	24.00±2.63	24.94±2.53
	Q_2	4.07±0.75	4.16±0.79	4.24±0.67	3.82±0.91	3.99±0.86	3.99±0.86
ClayFF	Q_4	66.47±3.23	66.58±2.72	67.00±2.80	67.74±2.21	67.98±1.87	67.82±1.83
	Q_3	29.82±2.54	29.71±1.76	29.38±2.27	28.48±1.76	28.64±1.23	28.89±1.40
	Q_2	3.62±1.00	3.54±0.93	3.46±0.92	3.70±1.07	3.29±0.76	3.13±0.65