Supplementary Material

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Table 1 shows the different sets of parameters from different sources that where used for simulating titrating silica surfaces with Faunus [6]. Tables 2–3 show the simulation results for the surface charge density and the ratio between simulated charge and the experimentally reported charge by Samoshina et al. [5] for ionic strengths of 10 and 100 mM, respectively. The charges were placed on a square lattice in the simulations.

On average, the surface charge density from simulations was 5.0 times the experimentally determined charge.

Parameter set	**pK_a 1**	**Percentage (%)**	**pK_a 2**	**Percentage (%)**	**Silanol group density ($Å^{-2}$)**
1 [4]	7.6	100	-	-	0.08
2 [3]	4.5	19	8.5	81	0.049
3 [2]	5.5	15	9.0	85	0.049
4 [1]	7.1	100	-	-	0.049

Table 1: The four sets of parameters that were used for titrating surface simulations and the references for the parameter sets. Some find that there are two types of silanol groups with different pK_a values while others find only one type of group.

Parameter set	**Charge density ($e/Å^2$)**	**Simulated charge/experimental**
1	-0.00198	3.17
2	-0.00477	7.64
3	-0.00318	5.09
4	-0.00238	3.81

Table 2: Charge densities found from titrating silica surface simulations at pH 7 and ionic strength 10 mM and their relation to the experimentally determined surface charge.

Parameter set	**Charge density ($e/Å^2$)**	**Simulated charge/experimental**
1	-0.00467	3.74
2	-0.00877	7.03
3	-0.00600	4.81
4	-0.00595	4.76

References

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