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Modeling of solid–liquid interfaces using scaled charges: rutile (110) surfaces

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Supporting Information

GROMACS SIMULATION SETUP

An archive file containing all Gromacs files with the force fields, configuration and parameter files for NaCl solution at nonhydroxylated rutile surface -0.4 C/m^2 with scaled charges is provided.

Setup for other systems is available upon request from the authors or available here: http://home.prf.jcu.cz/~predota/eccr-rutile

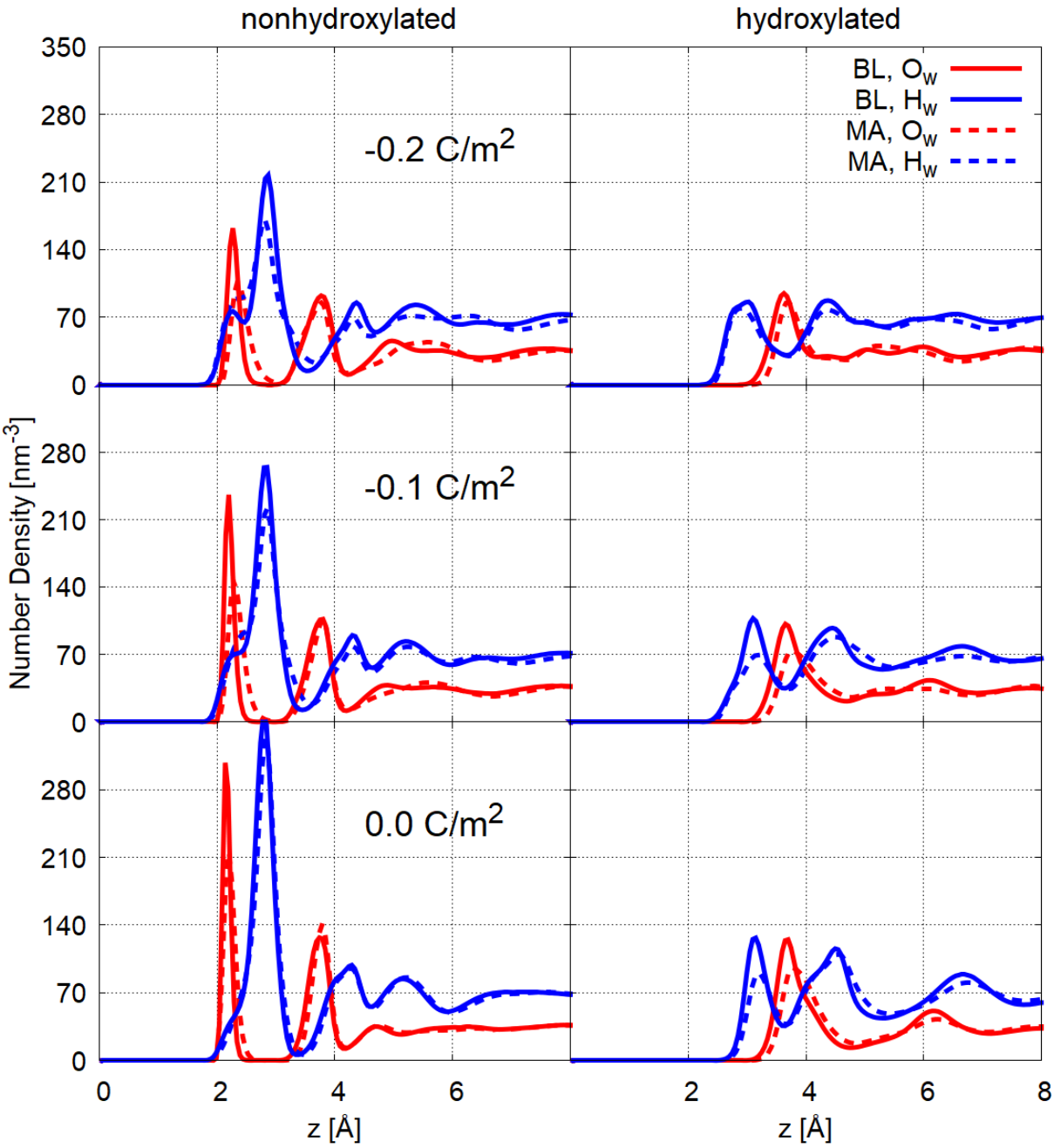

Figure S1. Comparison of water oxygen and water hydrogen axial density profiles from simulations at nonhydroxylated (left) and hydroxylated (right) surfaces with ≈0.4 M NaCl using Matsui-Akaogi (MA)[1] or Brandt and Lyabartsev (BL)[2] parameters.

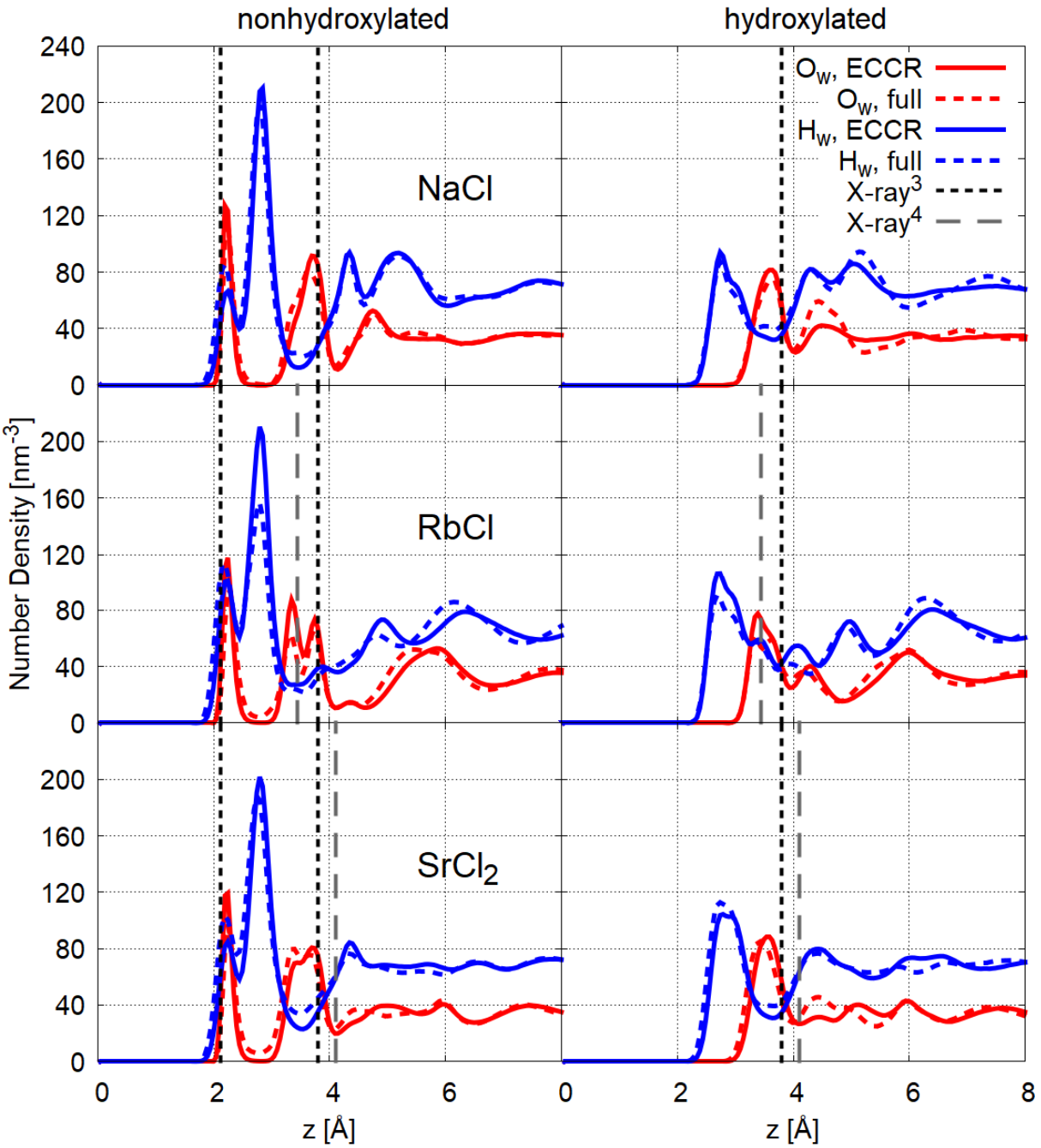

Figure S2. Axial number density profiles of water oxygens and water hydrogens from the system with the most negatively charged (σ = –0.416 C/m^2) nonhydroxylated (left) and hydroxylated (right) rutile surfaces in the presence of different salts. Comparison with X-ray data is shown for O_w from Refs 3 and 4, respectively.

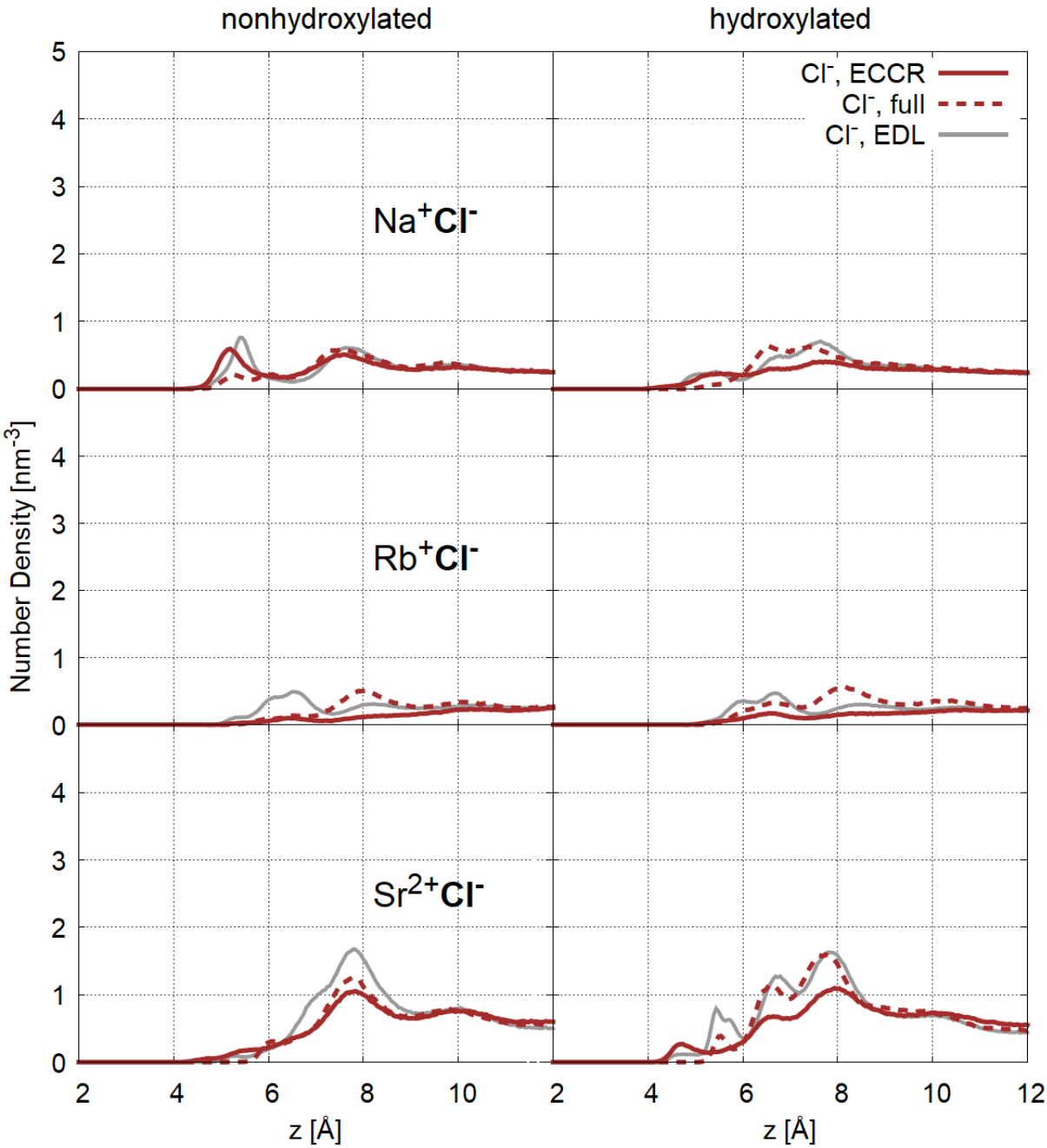

Figure S3. Axial number density profiles of chloride ions from the system with the most negatively charged (σ = –0.416 C/m^2) nonhydroxylated (left) and hydroxylated (right) rutile surfaces.

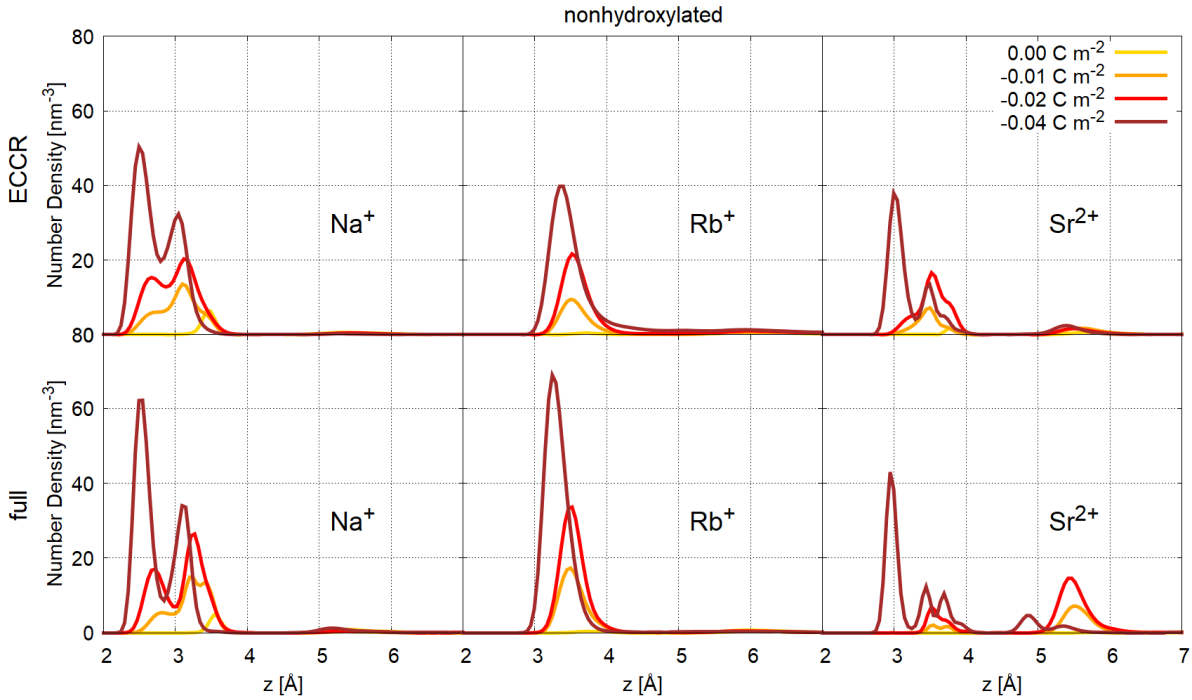

Figure S4. Axial number density profiles of cations at nonhydroxylated rutile surfaces of different surface charge densities with either 'ECCR' (top) or 'full' (bottom) model applied.

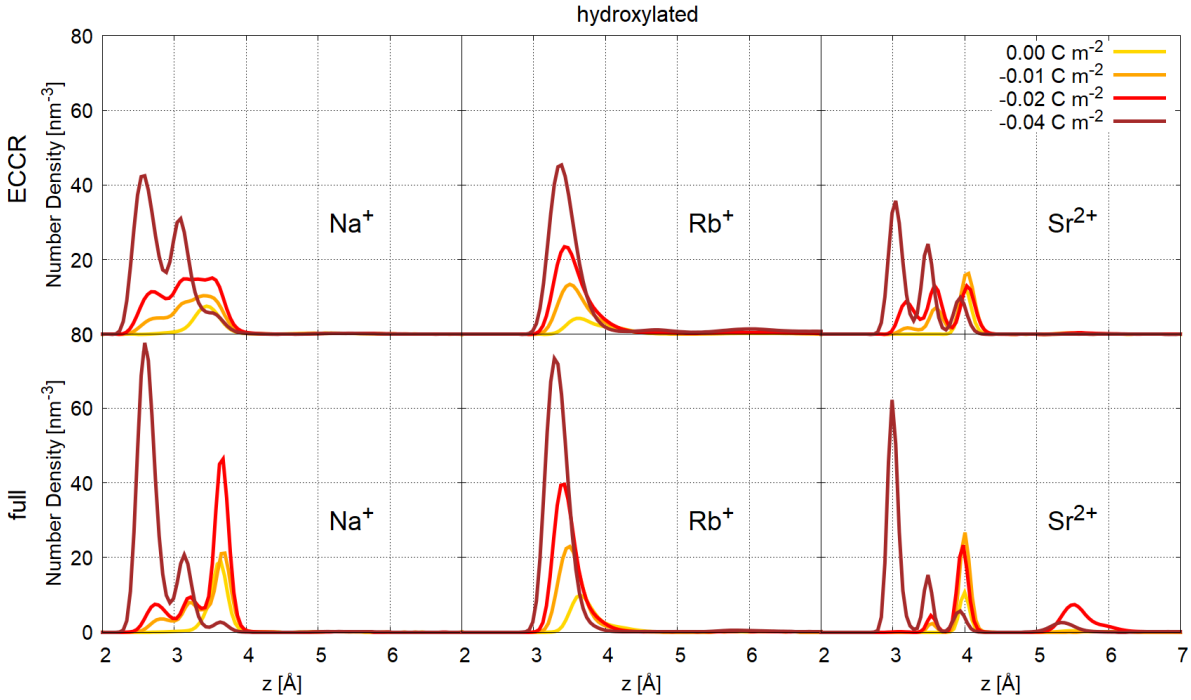

Figure S5. The same as S4, but at hydroxylated surface.

Table S1. Ion-Water Distances ($d_{\text{ion-O}}$) from Simulations and Experiment

ion	$d_{\text{ion-O}}$ (Å)			
	ECCR	full	EDL	experiment[a]
Na^+	2.30	2.37	2.45	2.39
Rb^+	2.91	2.89	2.93	2.91
Sr^{2+}	2.56	2.56	2.64	2.63
Cl^-	3.16	3.14	3.25	3.17

[a]Ion−water distance from Ref 5.

Table S2. Numbers of Ions in the Simulated Systems

surface charge density	surface charge [e]	Na^+	Rb^+	Sr^{2+}	Cl^-
0.000	0	18	18	13	18[a,b], 26[c]
−0.104	−18	30	30	22	12[a,b], 26[c]
−0.208	−36	51	48	31	15[a], 12[b], 26[c]
−0.416	−72	84	84	49	12[a,b], 26[c]

[a]For the system with Na^+. [b]For the system with Rb^+. [c]For the system with Sr^{2+}.

Table S3. Heights of the Cations (in Å) at the Adsorption Sites of the Most Charged (σ = –0.416 C/m^2) Rutile Surface[a]

ion	type	*nh-0.4*		*h-0.4*	
		ECCR	full	ECCR	full
Na^+	TD	**2.55**	**2.55**	**2.61**	**2.62**
	BOBO	*b*	2.54	2.63	2.62
	BOTO	**3.00**	**3.03**	**3.04**	**3.00**
	TOTO	*b*	*b*	3.54	*b*
Rb^+	TD	**3.43**	**3.30**	**3.42**	**3.34**
	BOBO	*b*	3.33	*b*	3.31
	BOTO	**3.69**	**3.34**	**3.59**	**3.36**
	TOTO	*b*	*b*	*b*	*b*
Sr^{2+}	TD	**3.03**	**2.97**	**3.05**	**3.01**
	BOBO	3.04	2.98	3.04	2.99
	BOTO	**3.44**	**3.41**	**3.49**	**3.50**
	TOTO	*b*	4.21	3.94	3.92

[a]Less occupied adsorption sites are included in this table. Predominant surface complexes are shown in bold. [b]A relative contribution of the adsorption site is lower than 3%.

References

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