

Supplementary Material for

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Effect of Hydration on the Intermolecular Interaction of Various Quaternary Ammonium Based Head groups with Hydroxide Ion of Anion Exchange Membrane Studied at the Molecular Level

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Table S1: Description for our designed systems at 298 K and 1 bar.

	QA	OH ⁻	H ₂ O	Number of atoms	Box size (nm ³)
(a)	1	1	3	39	2.5×2.5×2.5
(b)	1	1	3	45	2.5×2.5×2.5
(c)	1	1	3	38	2.5×2.5×2.5
(c)	1	1	9	56	2.5×2.5×2.5
(c)	1	1	15	74	2.5×2.5×2.5
(c)	1	1	500	1529	2.46×2.46×2.46
(c)	5	5	15	190	4.5×4.5×4.5
(c)	5	5	45	280	4.5×4.5×4.5
(c)	5	5	75	370	4.5×4.5×4.5
(d)	1	1	3	45	2.5×2.5×2.5
(e)	1	1	3	49	2.5×2.5×2.5
(f)	1	1	3	53	2.5×2.5×2.5
(f)	1	1	9	71	2.5×2.5×2.5
(f)	1	1	15	89	2.5×2.5×2.5
(f)	1	1	500	1544	2.47×2.47×2.47
(f)	5	5	15	265	4.5×4.5×4.5
(f)	5	5	45	355	4.5×4.5×4.5
(f)	5	5	75	445	4.5×4.5×4.5