SUPPLEMENTARY MATERIALS

Exchange Mechanism of Alkaline and Alkalineearth Elements in Zeolite N

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Table S1. The Mulliken partial cherges, force field assigned types and number of framework, extra-framework and water atoms used in this study.

Atom	Atomic charges	Force fields assigned	Number of atoms	
			(001)	(110)
Si 1	1.756	si4z	16	16
Si 2	1.718	si4z	64	64
Al 1	1.654	al4z	16	16
Al 2	1.623	al4z	64	64
O	-1.0886	o2z	304	312
O_{-OH}	-0.8453	o2z	32	16
H_{-OH}	0.299	h1o	32	16
K1	+1	k+	32	32
K2	+1	k+	64	64
Cl	-1	cl+	16	16
O_W	-0.82	o2*	128	128
H_W	0.41	h1o	256	256

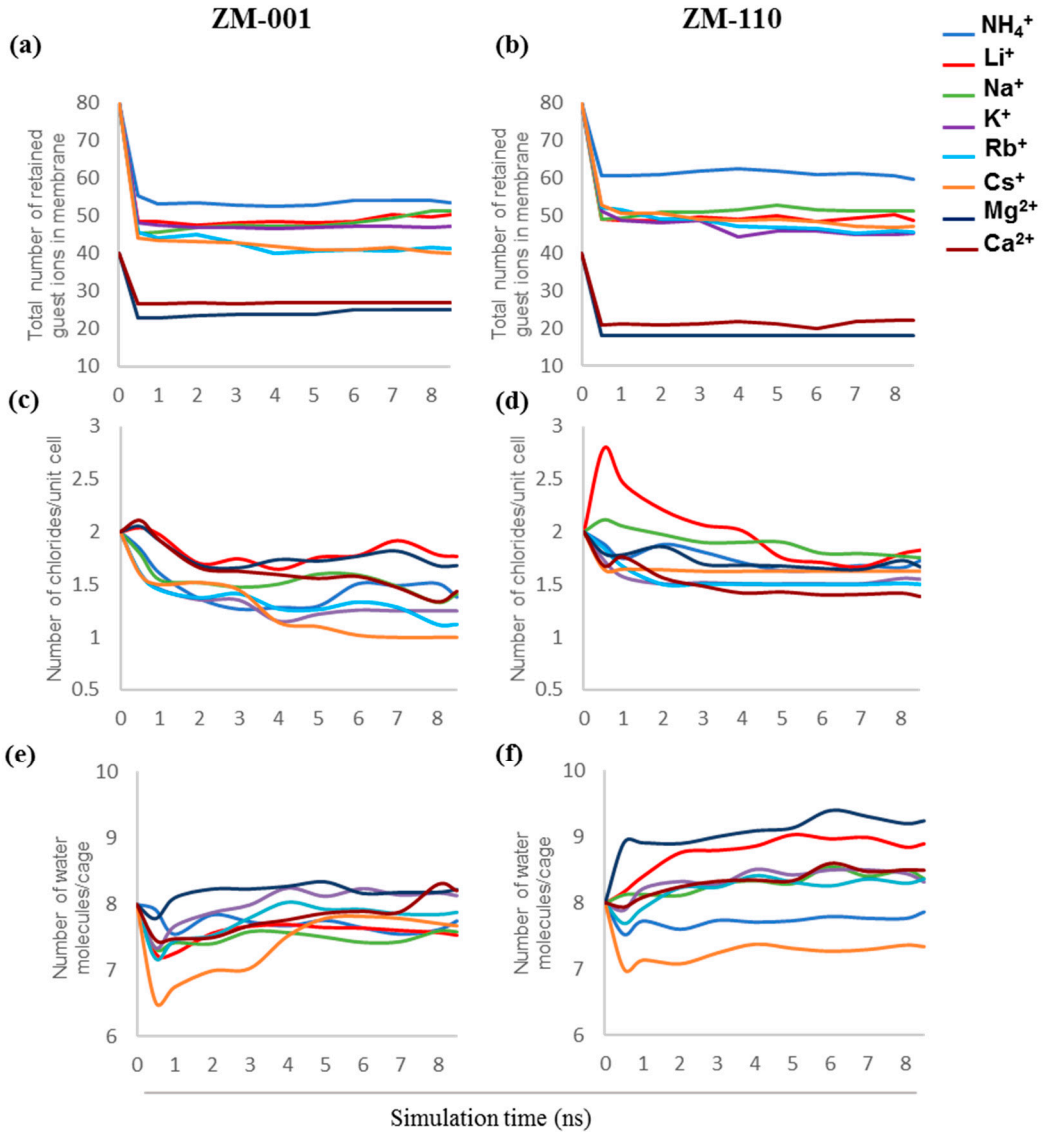


Figure S1. The retention of guest cations in (a) ZM-001 and (b) ZM-110, the number of retained chlorides and per unit cell of (c) ZM-001 and (e) ZM-110; ZM-001 and number of remained water molecules in each cage of (d) ZM-001 and (f) ZM-110.

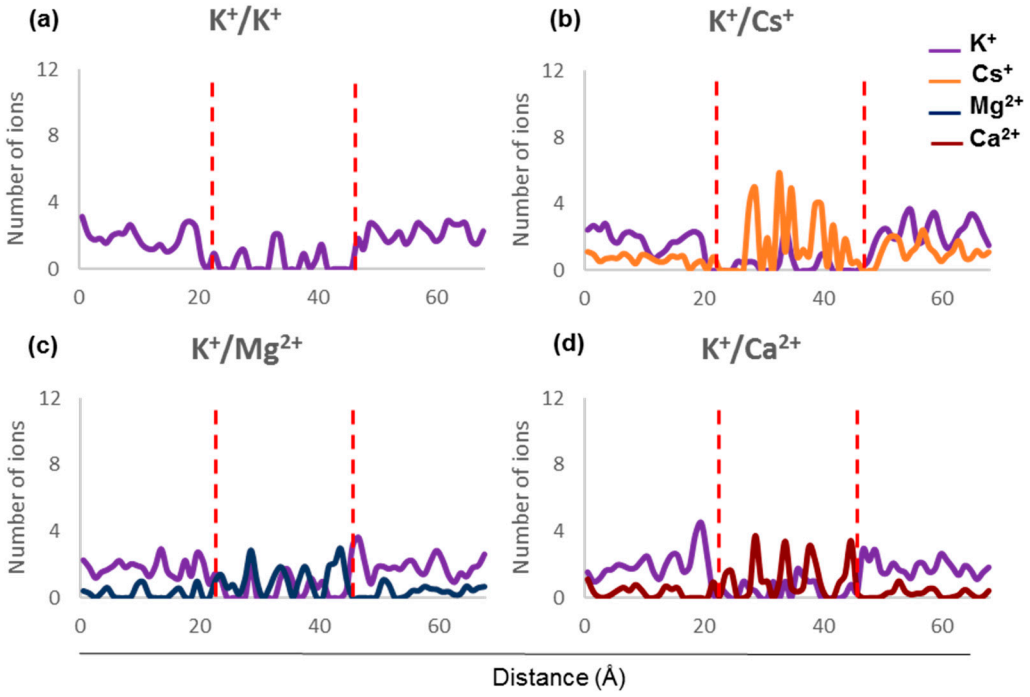


Figure S2. (a-d) ion concentration profiles along *z* direction after 8.5 ns MD simulations. The two red dashed lines indicate the location of ZM-001 surfaces in electrolyte solution.

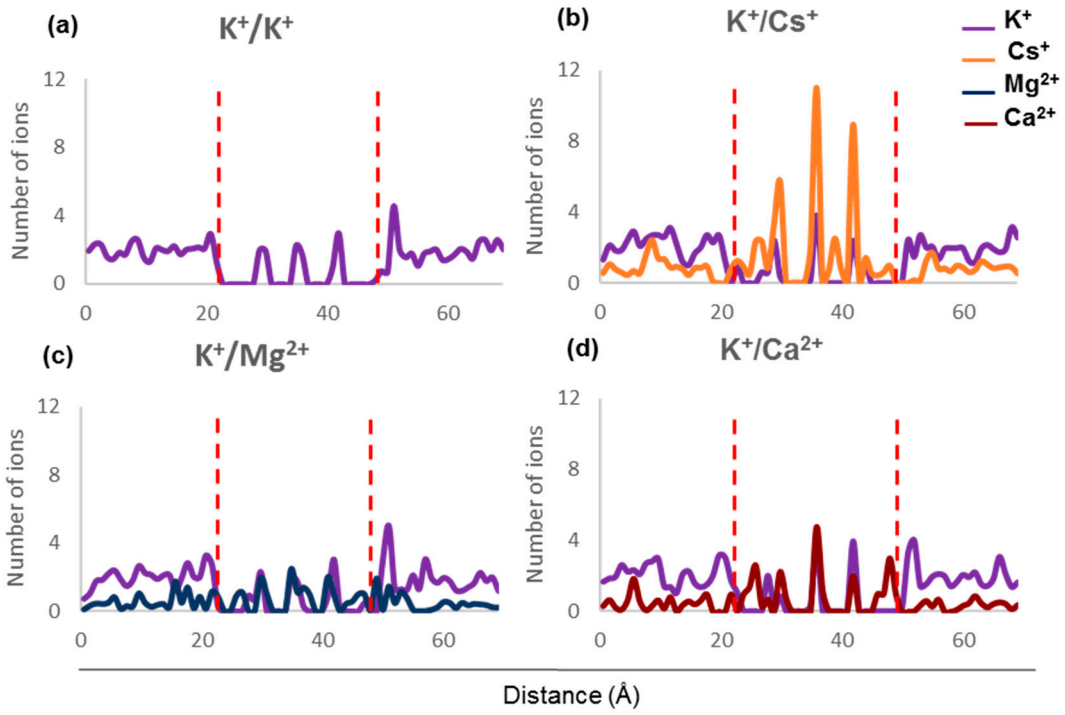


Figure S3. (a-d) ion concentration profiles along *z* direction after 8.5 ns MD simulations. The two red dashed lines indicate the location of ZM-110 surfaces in electrolyte solution.

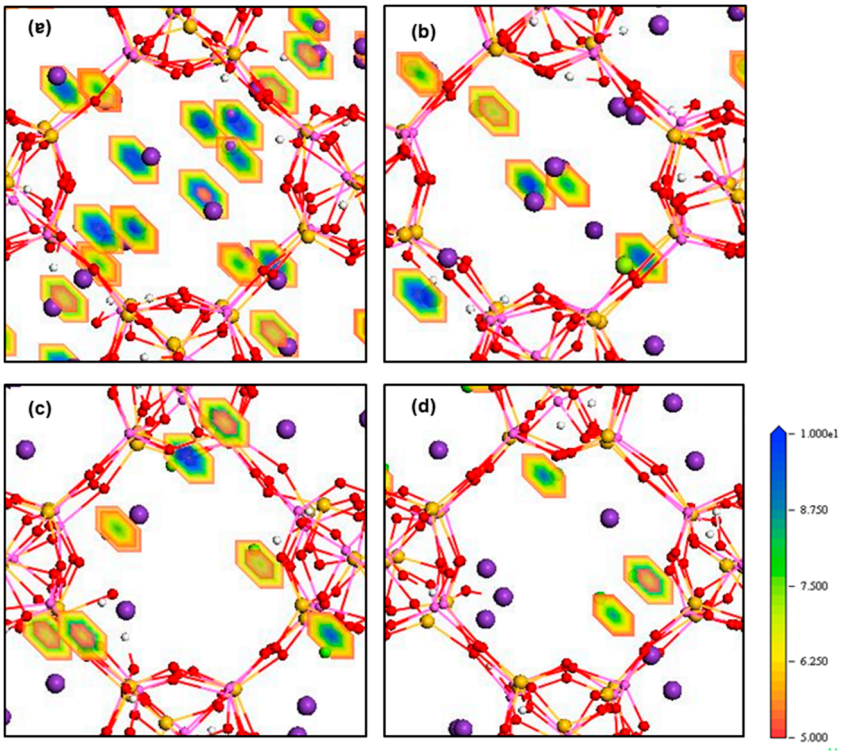
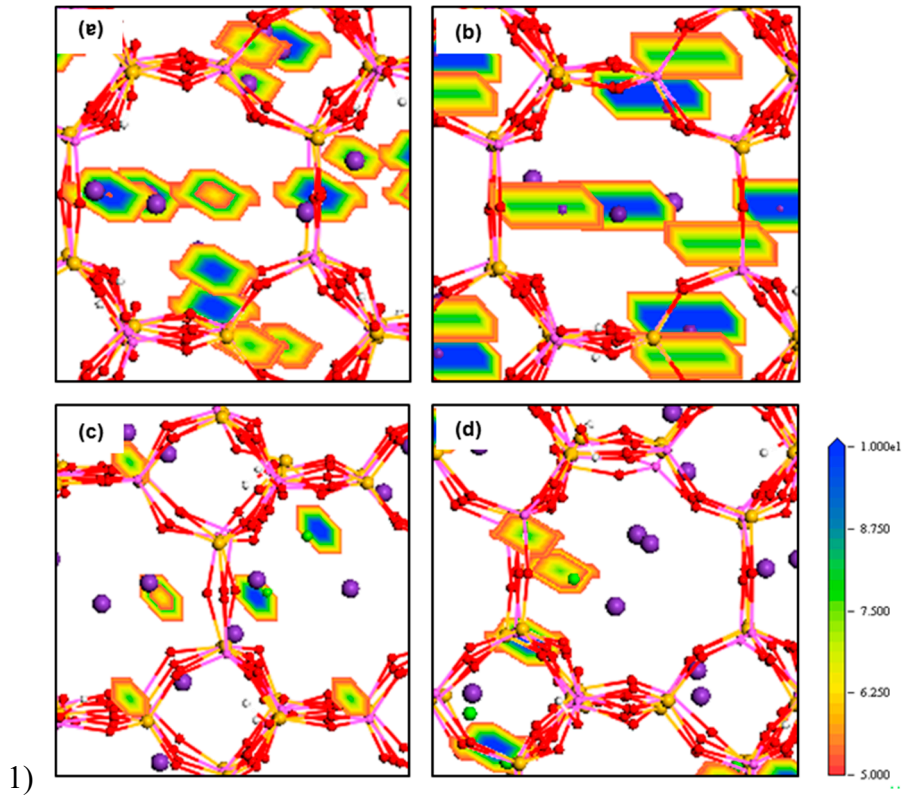


Figure S4. Density field maps of (a) K^+ in K^+/ K^+ system and M^n guest cations in (b) K^+/Rb^+, (c) K^+/Mg^{2+} and (d) K^+/Ca^{2+} systems retained inside ZM-001 after 8.5 ns MD simulations.



1)

Figure S5. Density field maps of (a) K^+ in K^+/ K^+ system and M^n guest cations in (b) K^+/Rb^+, (c) K^+/Mg^{2+} and (d) K^+/Ca^{2+} systems retained inside ZM-110 after 8.5 ns MD simulations.

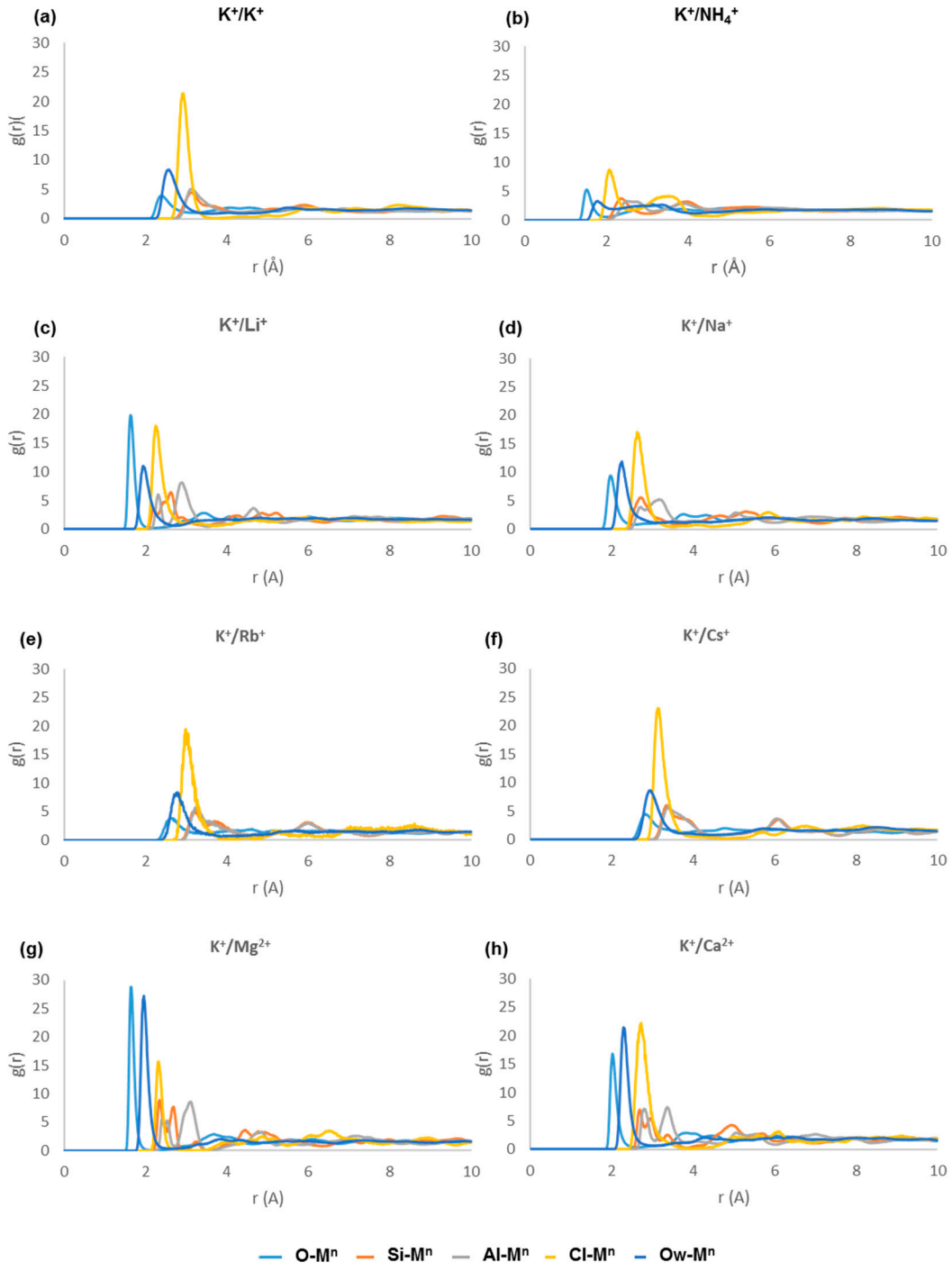


Figure S6. RDFs, g(r) for guest cations to framework atoms, chlorides and water molecules inside ZM-001 membrane.

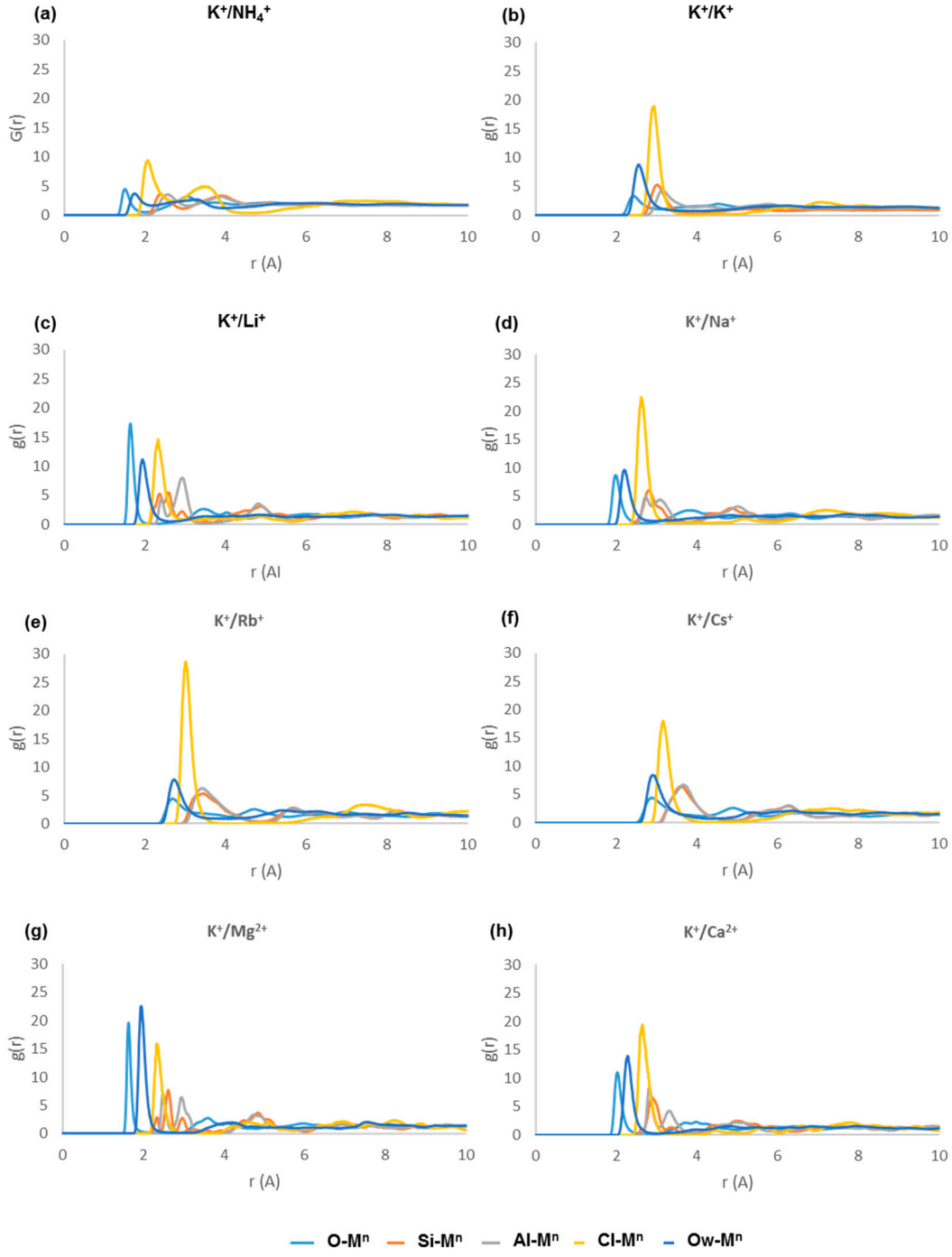


Figure S7. RDFs, g(r) for guest cations to framework atoms, chlorides and water molecules inside ZM-110 membrane.

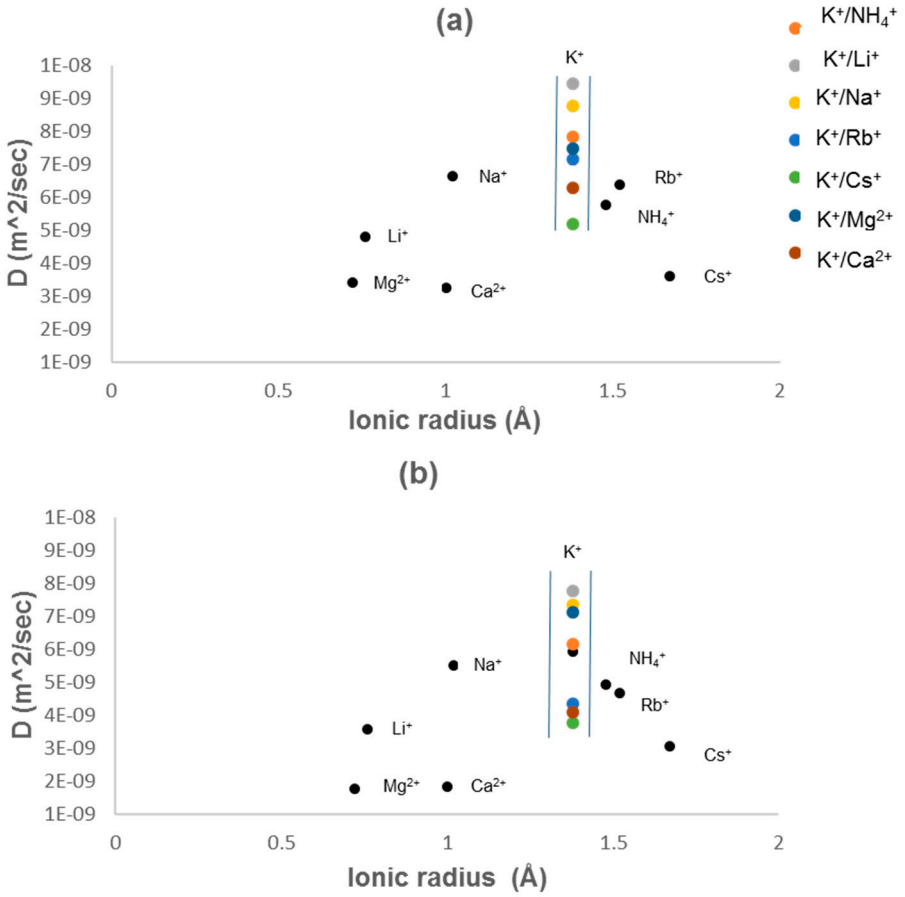


Figure S8. Self-diffusion coefficient of ions (D) inside electrolyte vs. ionic radius. The black labelled points are D values of guest cation in each system. The D values of K cations in electrolyte of each system are identified with different colours.

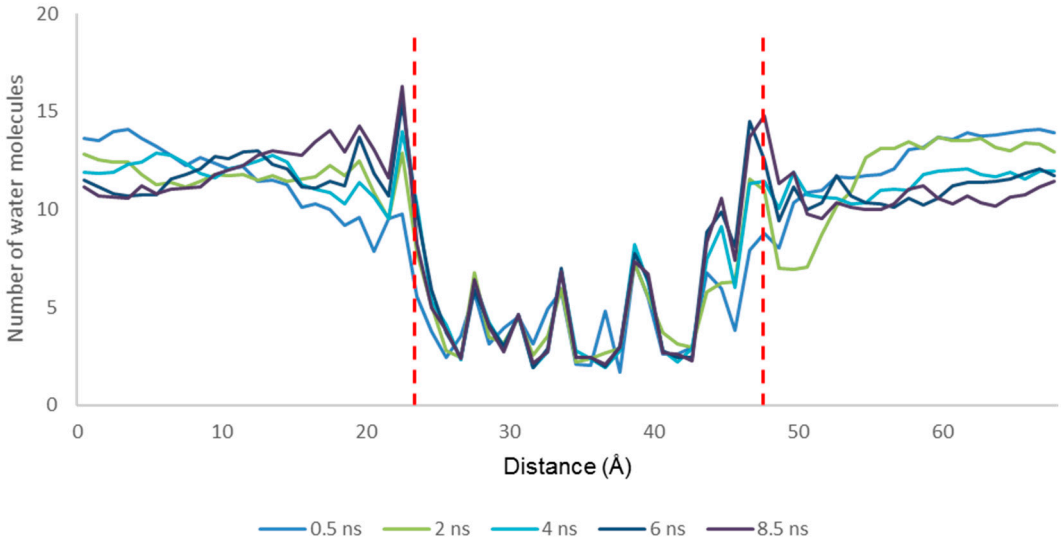


Figure S9. The concentration profile of water molecules along *z* direction for different times of MD simulations for K^+/Cs^+ system of ZM-001. The two red dashed lines indicate the location of ZM-001 surfaces in electrolyte solution.