Supporting Information

"Channel" or "Container"? Effect of the Pore Structure on Ion Transport in Porous MXene Electrodes

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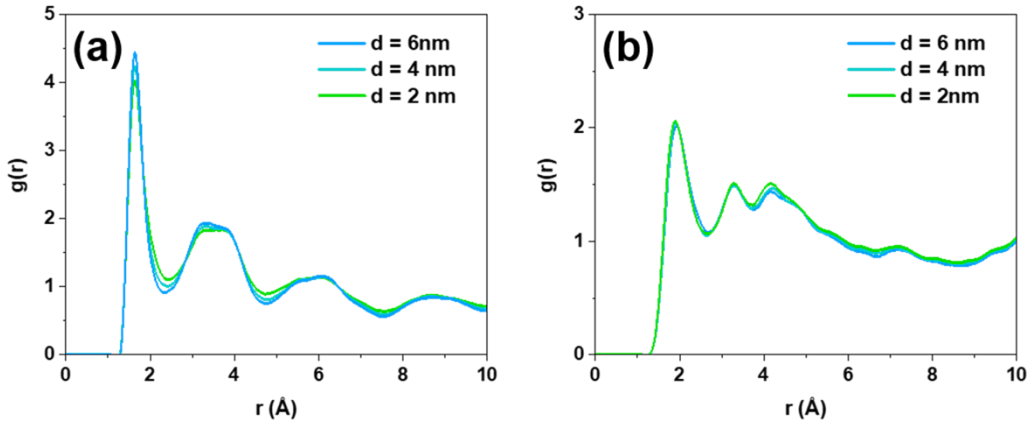

Fig. S1 Radial Distribution Function between the electrode surface of the and the electrolyte ions, (a) positive electrode，-OH groups - $[Tf_2N]^-$, (b) negative electrode, -OH groups - $[Emim]^+$. The H atoms in the -OH groups on the electrode surface, the H atoms in the alkyl group of $[Emim]^+$, and the O atoms in $[Tf_2N]^-$ were selected for analysis.

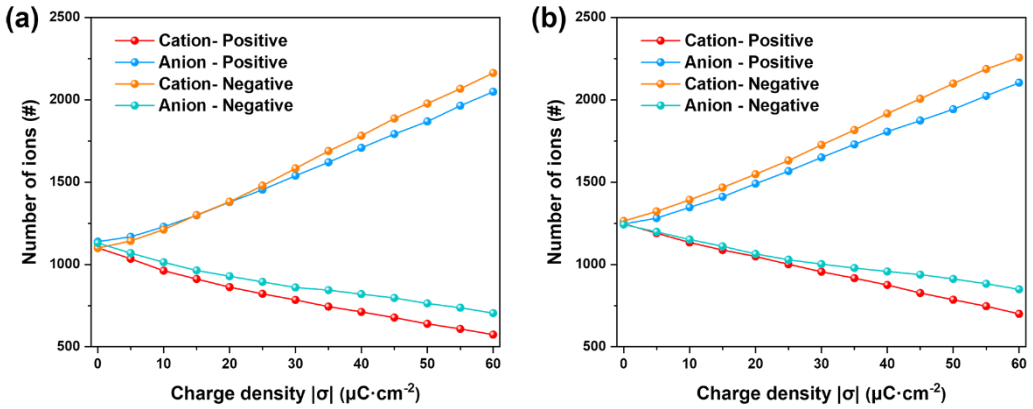

Fig. S2 Number change curve of the ions in the electrode during charging, (a) d = 2 nm, (b) d = 4nm.

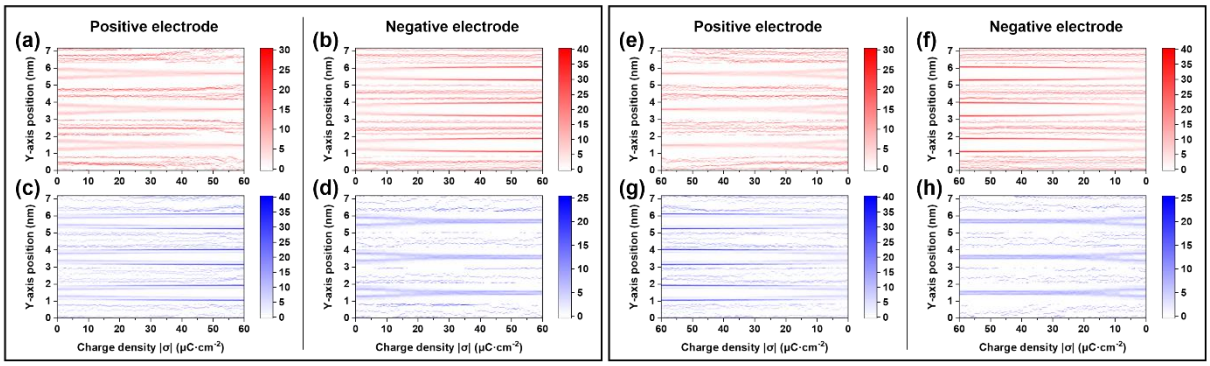

Fig. S3 Evolution of ion number density distribution within interlayers and pore structures of the electrode (d = 2 nm), (a-d) Charging process, (e-h) Discharge process, (a)(e) Cations in the positive electrode; (b)(f) Cations in the negative electrode; (c)(g) Anions in the positive electrode; (d)(h) Anions in the negative electrode.

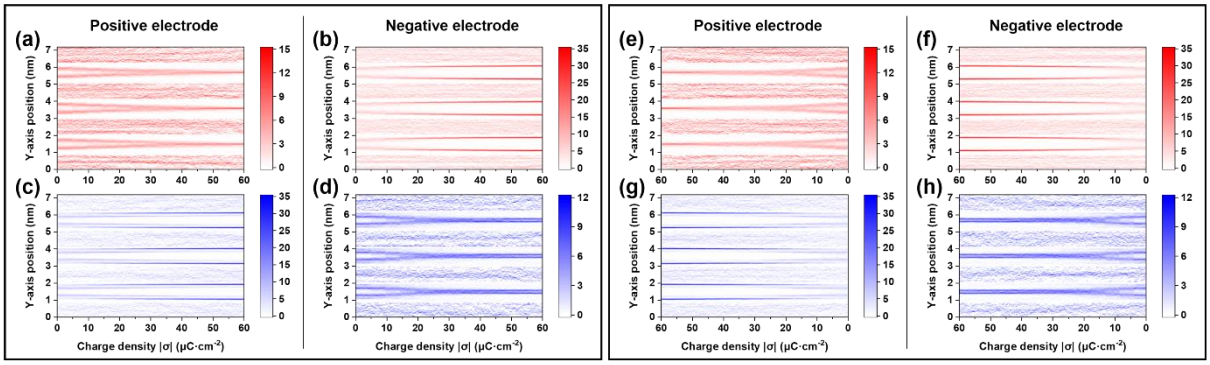

Fig. S4 Evolution of ion number density distribution within interlayers and pore structures of the electrode (d = 4 nm), (a-d) Charging process, (e-h) Discharge process, (a)(e) Cations in the positive electrode; (b)(f) Cations in the negative electrode; (c)(g) Anions in the positive electrode; (d)(h) Anions in the negative electrode.

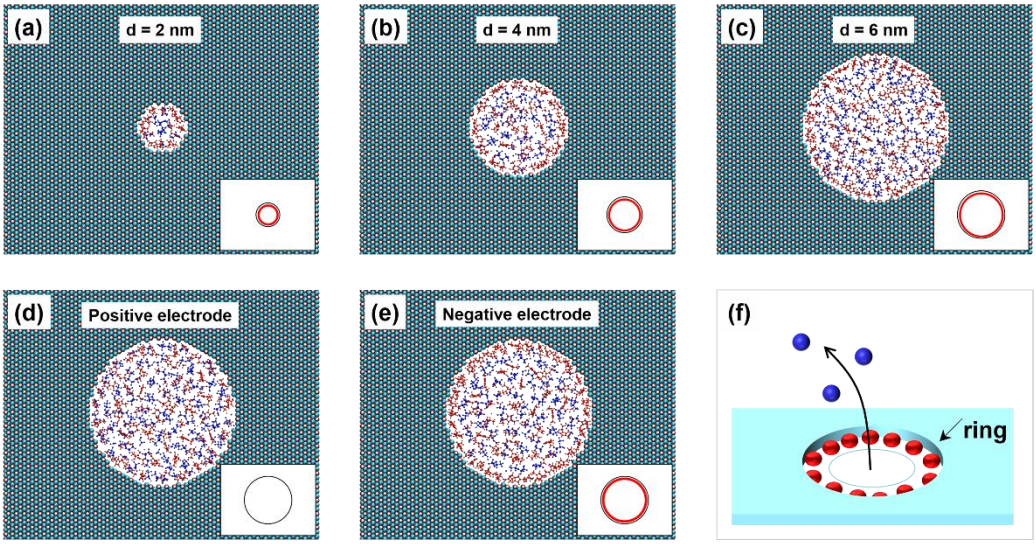

Fig. S5 Screenshots of ion distribution in different pores and diagram of the effective "Through-Pore" path, (a-c) $|\sigma| = 0$ μC·cm^{-2}, (d-e) $|\sigma| = 60$ μC·cm^{-2}, d = 6 nm. Cations are highlighted in red, and anions are highlighted in blue.

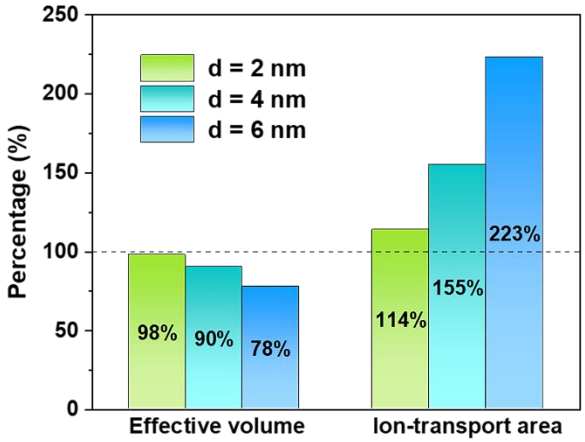

Fig. S6 Comparison of effective volume and ion-accessible surface area for electrodes with different pore sizes, based on their relative changes compared to electrodes of the same size without pores.

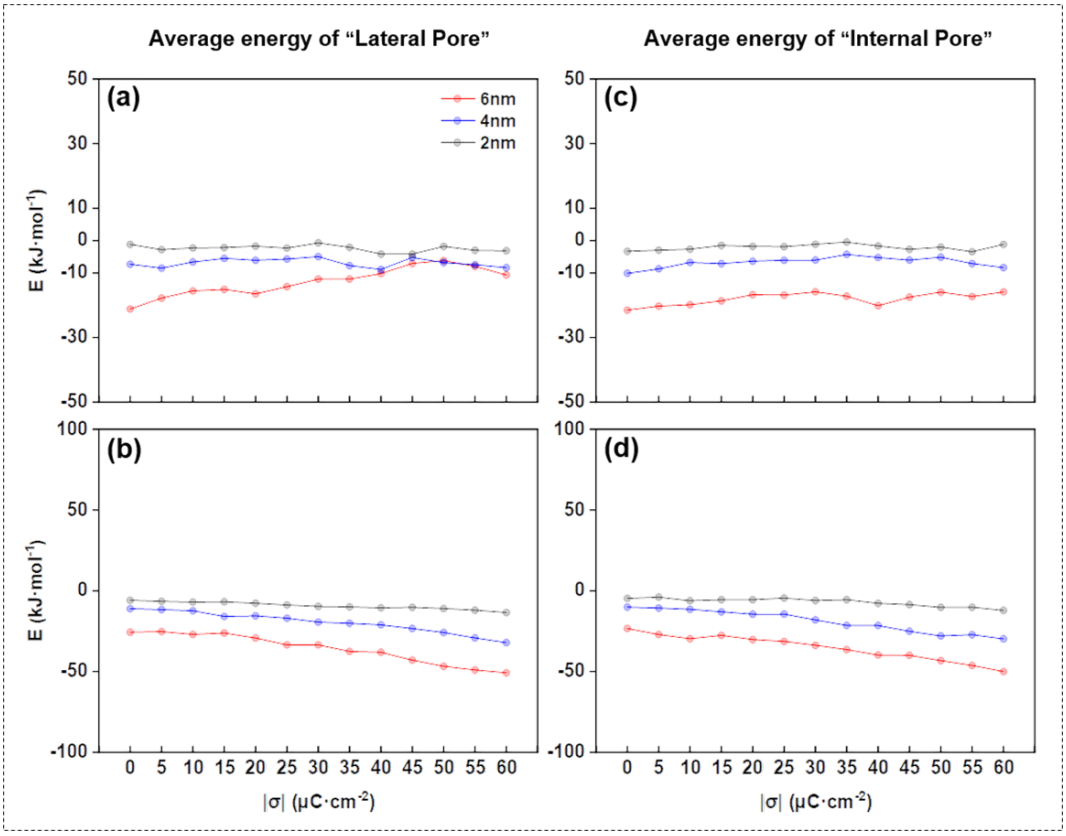

Fig. S7 Energy change curve between electrolyte ions in pores and electrodes of different groups during charging process. (a) Electrolyte ions in "Lateral Pore" with positive electrodes; (b) Electrolyte ions in "Lateral Pore" with negative electrodes; (c) Electrolyte ions in "Internal Pore" with positive electrodes; (d) Electrolyte ions in "Internal Pore" with negative electrodes.