

Rational Design of Solid Polymer Electrolyte based on Ionic Liquid Monomer for Supercapacitor Applications via Molecular Dynamics Study

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Supplementary Information

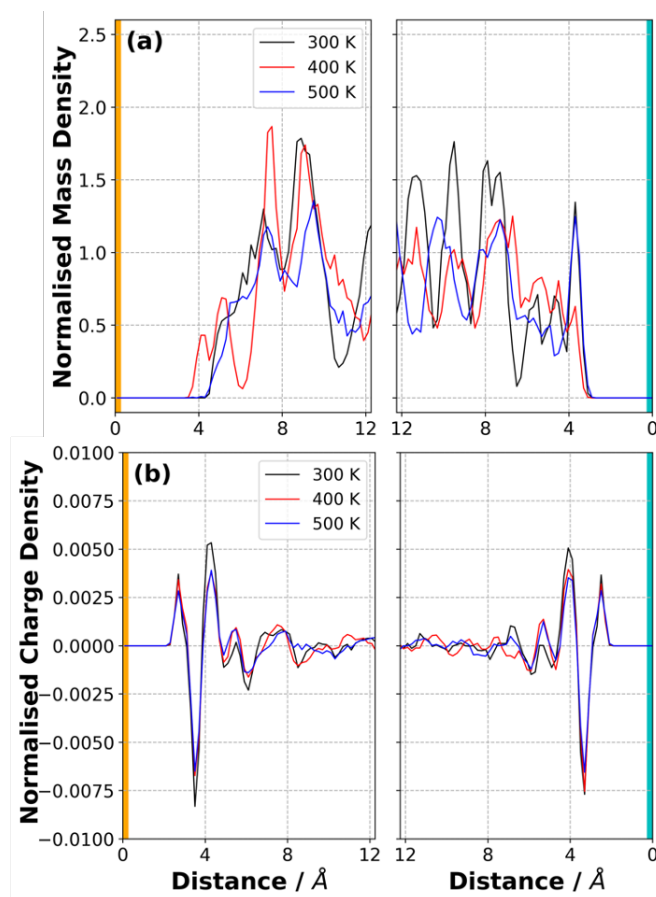


Figure S1: (a) Normalised mass density distribution of the reacted C atoms of cations at various temperatures. (b) Normalised charge density distribution near the negative (red bar) and positive (blue bar) electrodes obtained at the completion of the equilibration process of the polymerised samples at varying temperatures. No potential difference across the simulation cell was applied.

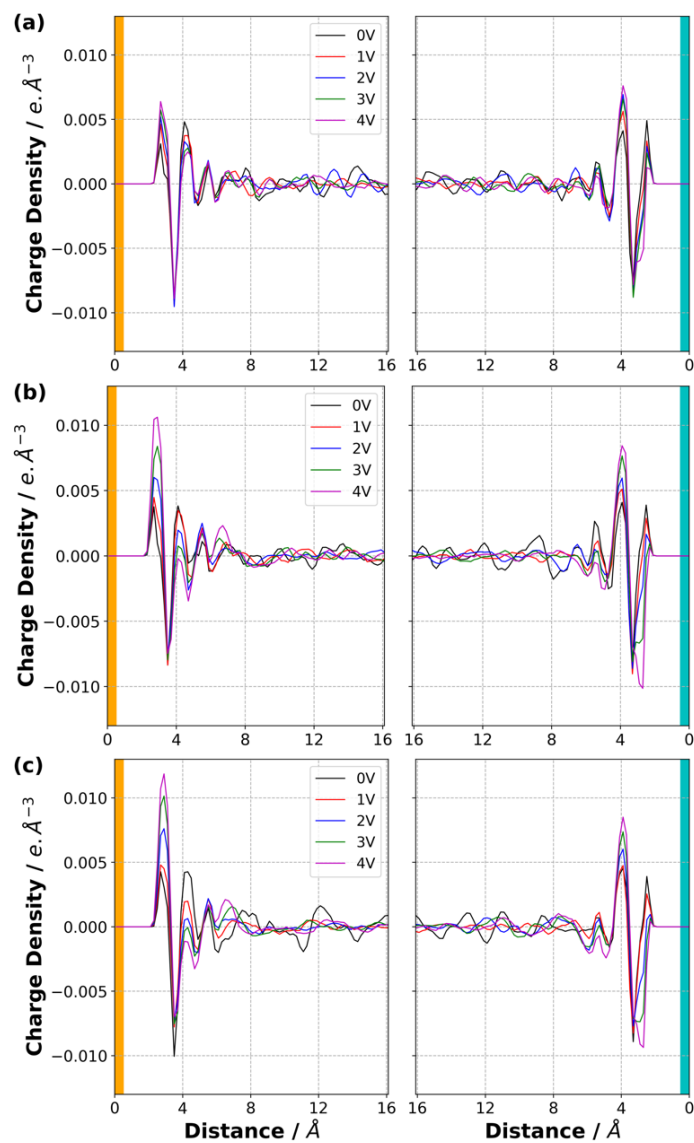


Figure S2: (a) Charge density distribution in the solid polymer electrolyte (SPE) at various $\Delta\Psi$ at (a) 300 K, (b) 400 K and (c) 500 K.

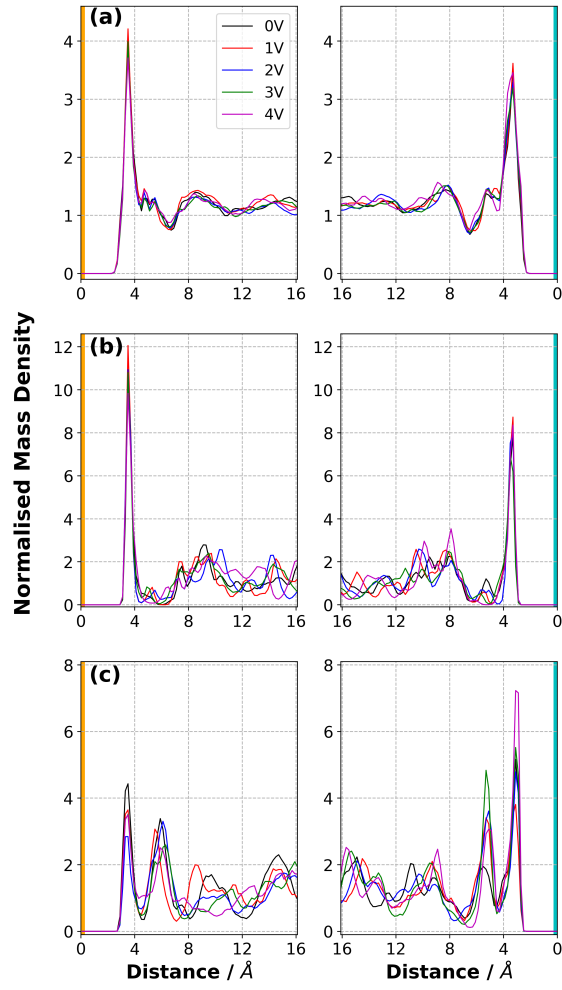


Figure S3: (a) Normalised mass density distribution of the (a) the entire SPE, (b) cations of the SPE, (c) anions at 300 K at various $\Delta\Psi$.

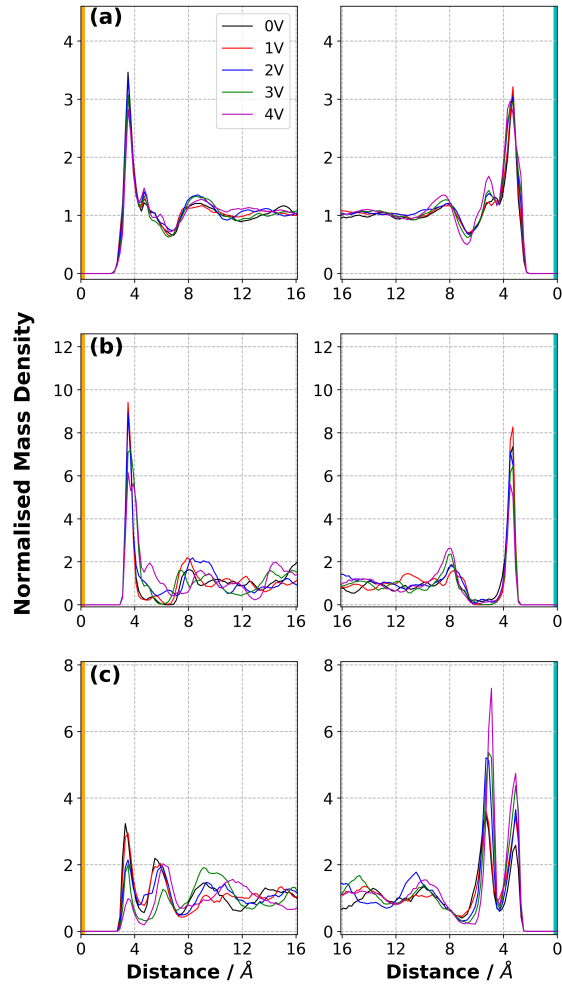


Figure S4: (a) Normalised mass density distribution of the (a) the entire SPE, (b) cations of the SPE, (c) anions at 400 K at various $\Delta\Psi$.

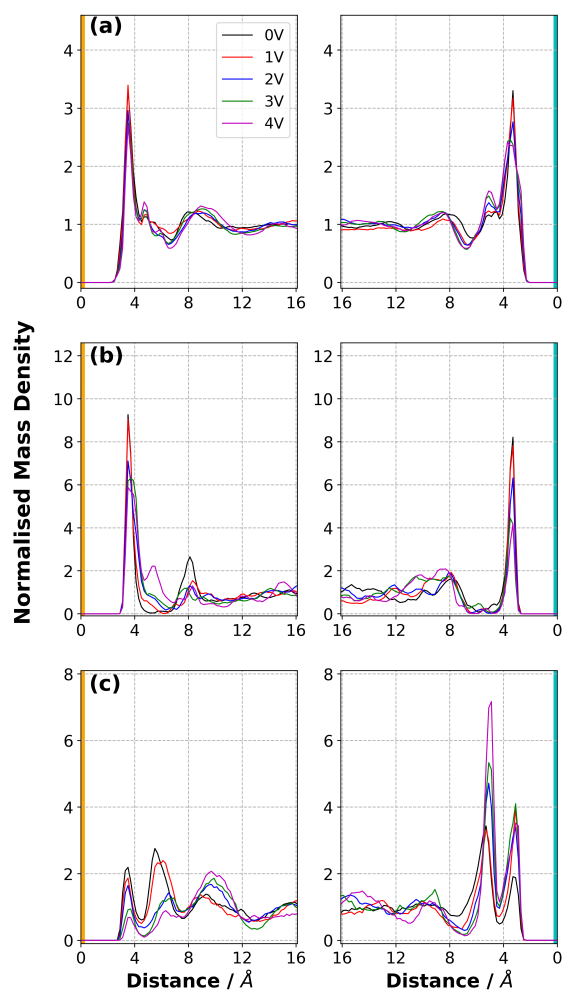


Figure S5: (a) Normalised mass density distribution of the (a) the entire SPE, (b) cations of the SPE, (c) anions at 500 K at various $\Delta\Psi$.

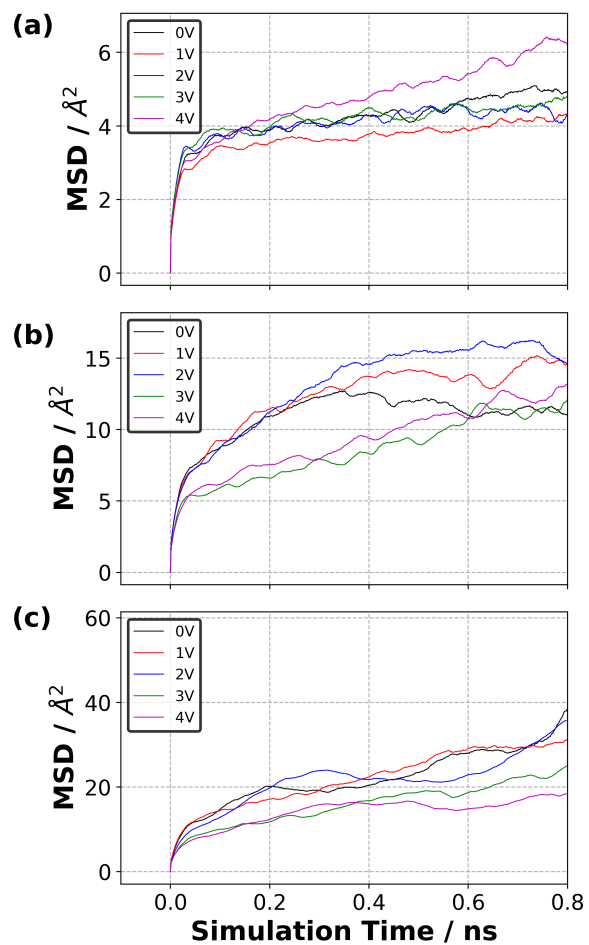


Figure S6: Mean square displacement (MSD) curves for the anion found in the electric double layer (EDL) (the thickness of 10 \AA from the negative electrode) obtained at different potential difference and temperatures: (a) 300 K, (b) 400 K and (c) 500 K.