Electronic Supplementary Material (ESI) for Soft Matter.

Supplementary Materials

Structure and dynamics of ions in dipolar solvents: a coarse-grained simulation study

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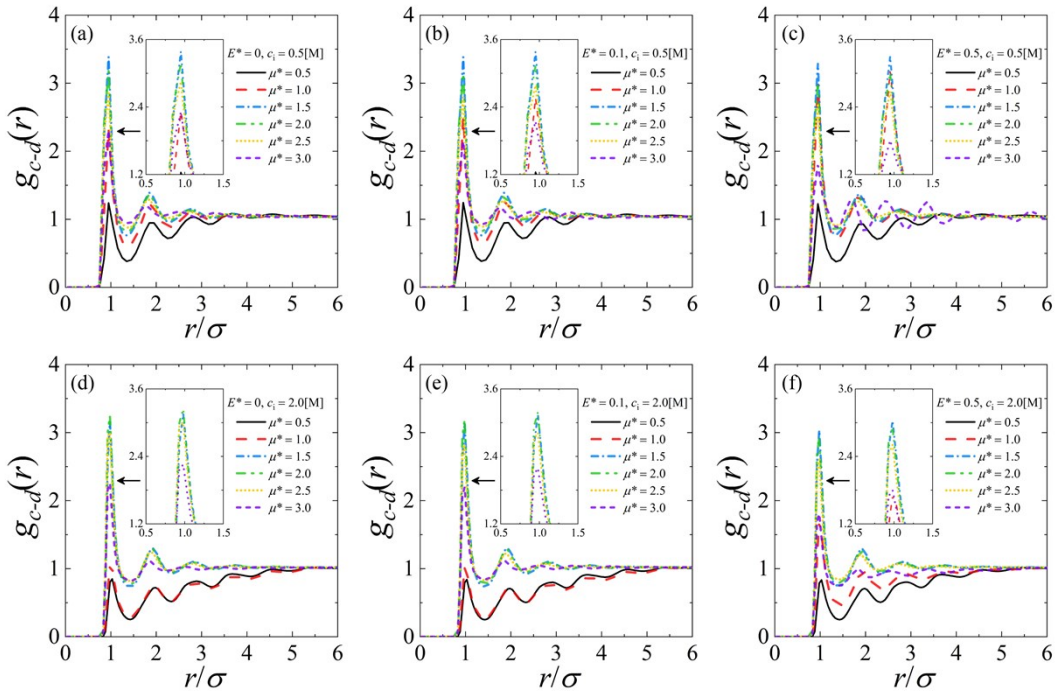

Fig. S1 Radial distribution functions of dipoles around each cation [$g_{c\text{-}d}(r)$] at different dipole moments (μ^*), ionic concentrations (c_i) and magnitudes of the external electrostatic field (E^*). The line colors correspond to the values of the dipole moments. (a) c_i = 0.5 [M], E^* = 0, (b) c_i = 0.5 [M], E^* = 0.1, (c) c_i = 0.5 [M], E^* = 0.5, (d) c_i = 2.0 [M], E^* = 0, (e) c_i = 2.0 [M], E^* = 0.1, and (f) c_i = 2.0 [M], E^* = 0.5.

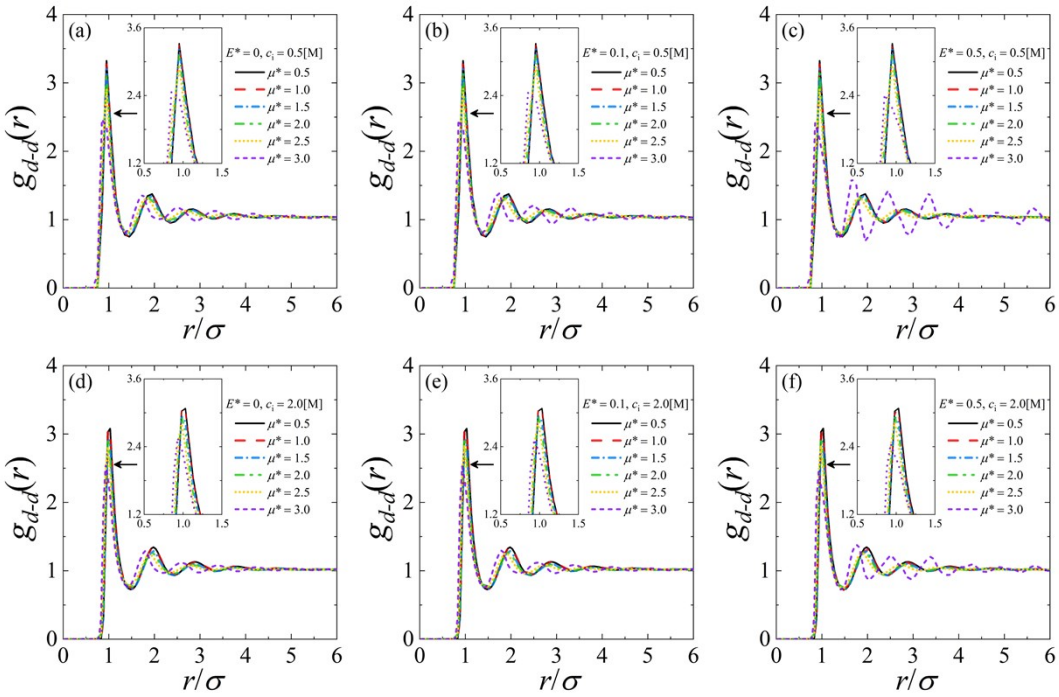

Fig. S2 Radial distribution functions of dipoles around each dipole [$g_{d\text{-}d}(r)$] at different dipole moments (μ^*), ionic concentrations (c_i) and magnitudes of the external electrostatic field (E^*). The line colors

correspond to the values of the dipole moments. (a) c_i = 0.5 [M], E^* = 0, (b) c_i = 0.5 [M], E^* = 0.1, (c) c_i = 0.5 [M], E^* = 0.5, (d) c_i = 2.0 [M], E^* = 0, (e) c_i = 2.0 [M], E^* = 0.1, and (f) c_i = 2.0 [M], E^* = 0.5.

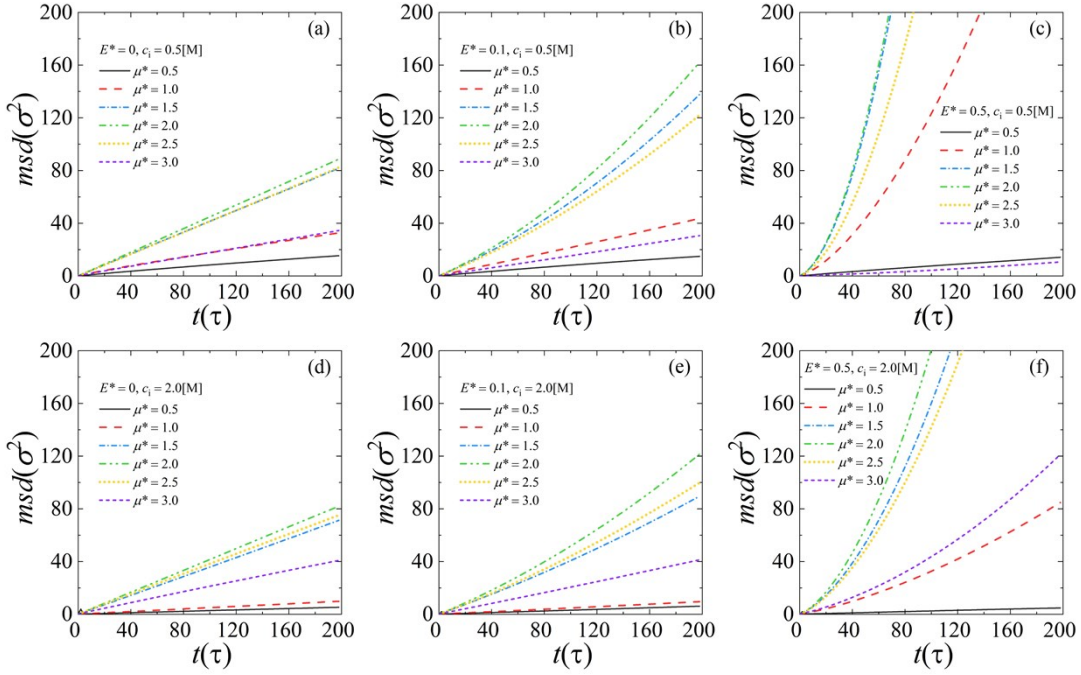

Fig. S3 Mean-squared displacement of cations as a function of simulation time. The line colors correspond to the values of the dipole moments. (a) c_i = 0.5 [M], E^* = 0, (b) c_i = 0.5 [M], E^* = 0.1, (c) c_i = 0.5 [M], E^* = 0.5, (d) c_i = 2.0 [M], E^* = 0, (e) c_i = 2.0 [M], E^* = 0.1, and (f) c_i = 2.0 [M], E^* = 0.5.

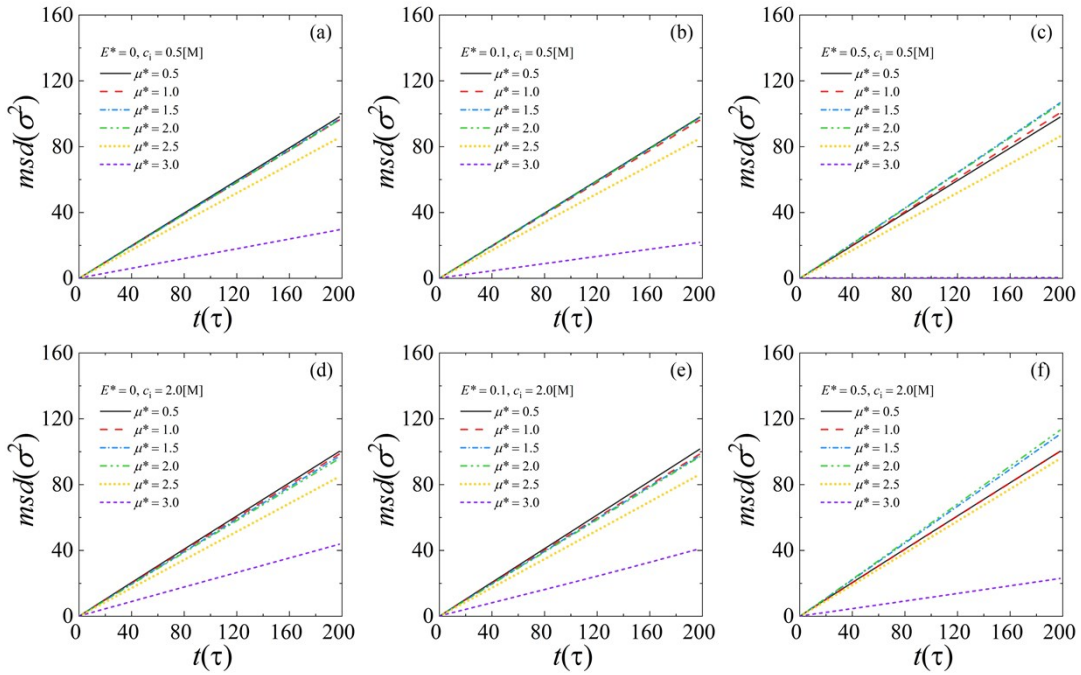

Fig. S4 Mean-squared displacement of dipoles as a function of simulation time. The line colors correspond to the values of the dipole moments. (a) c_i = 0.5 [M], E^* = 0, (b) c_i = 0.5 [M], E^* = 0.1, (c) c_i = 0.5 [M], E^* = 0.5, (d) c_i = 2.0 [M], E^* = 0, (e) c_i = 2.0 [M], E^* = 0.1, and (f) c_i = 2.0 [M], E^* = 0.5.

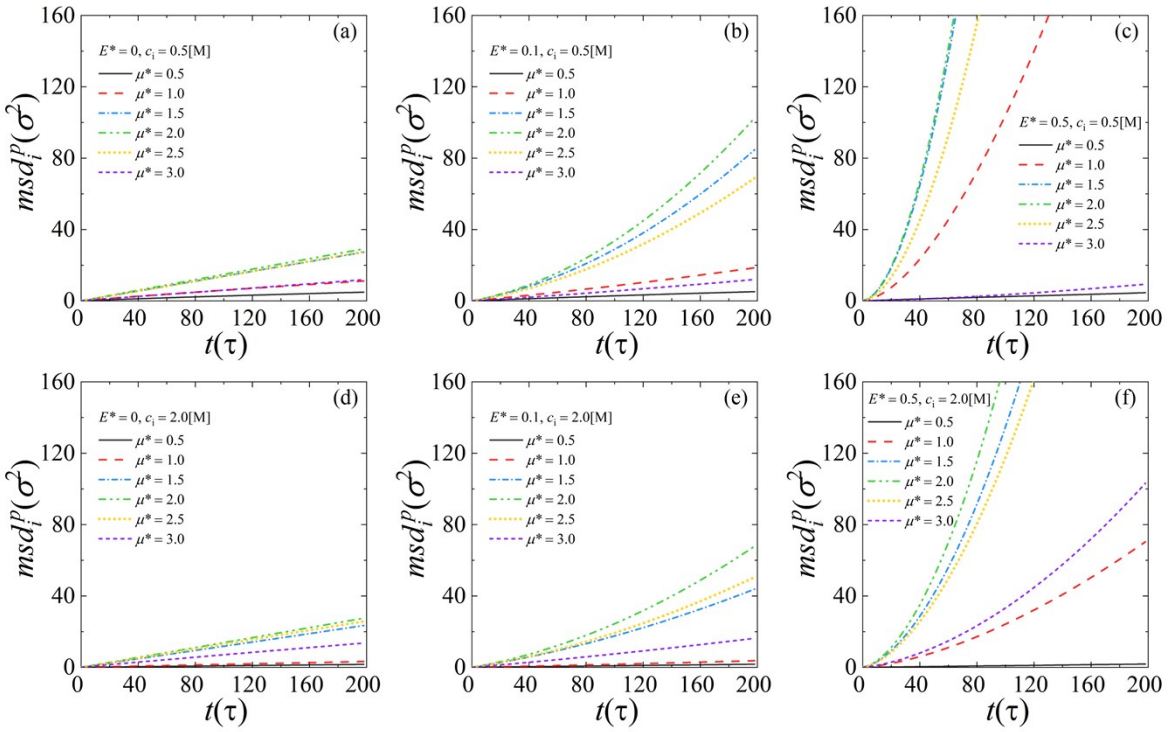

Fig. S5 The components of Mean-squared displacement of cations in directions parallel to the electric field as a function of simulation time. The line colors correspond to the values of the dipole moments. (a) c_i = 0.5 [M], E^* = 0, (b) c_i = 0.5 [M], E^* = 0.1, (c) c_i = 0.5 [M], E^* = 0.5, (d) c_i = 2.0 [M], E^* = 0, (e) c_i = 2.0 [M], E^* = 0.1, and (f) c_i = 2.0 [M], E^* = 0.5.

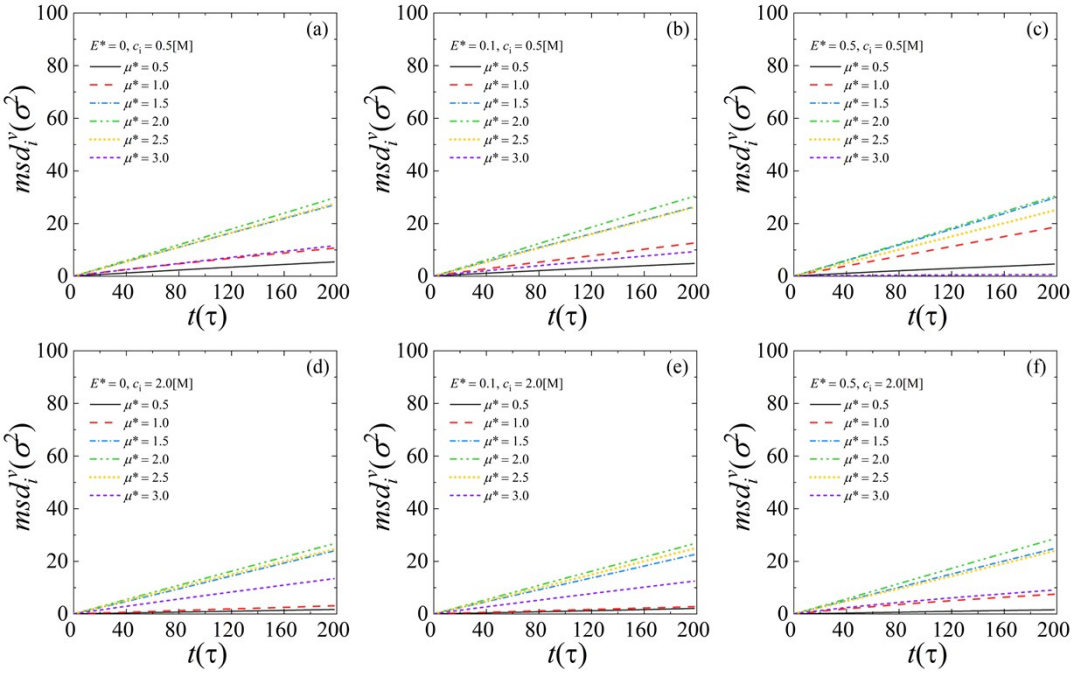

Fig. S6 The components of Mean-squared displacement of cations in directions vertical to the electric field as a function of simulation time. The line colors correspond to the values of the dipole moments. (a) c_i =

0.5 [M], E^* = 0, (b) c_i = 0.5 [M], E^* = 0.1, (c) c_i = 0.5 [M], E^* = 0.5, (d) c_i = 2.0 [M], E^* = 0, (e) c_i = 2.0 [M], E^* = 0.1, and (f) c_i = 2.0 [M], E^* = 0.5.

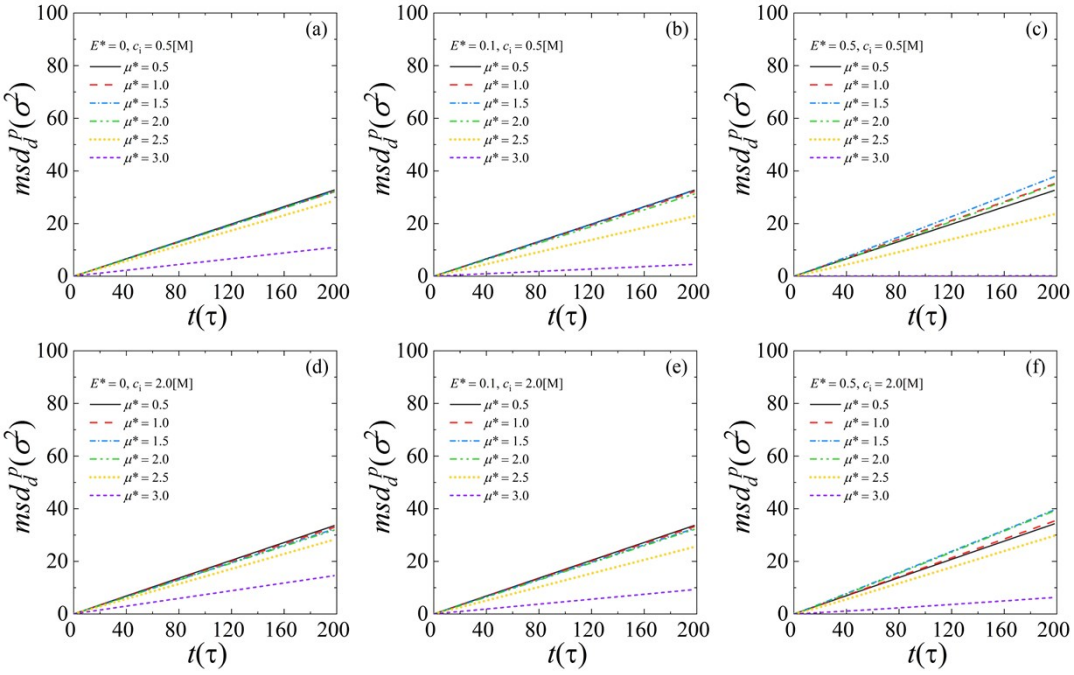

Fig. S7 The components of Mean-squared displacement of dipoles in directions parallel to the electric field as a function of simulation time. The line colors correspond to the values of the dipole moments. (a) c_i = 0.5 [M], E^* = 0, (b) c_i = 0.5 [M], E^* = 0.1, (c) c_i = 0.5 [M], E^* = 0.5, (d) c_i = 2.0 [M], E^* = 0, (e) c_i = 2.0 [M], E^* = 0.1, and (f) c_i = 2.0 [M], E^* = 0.5.

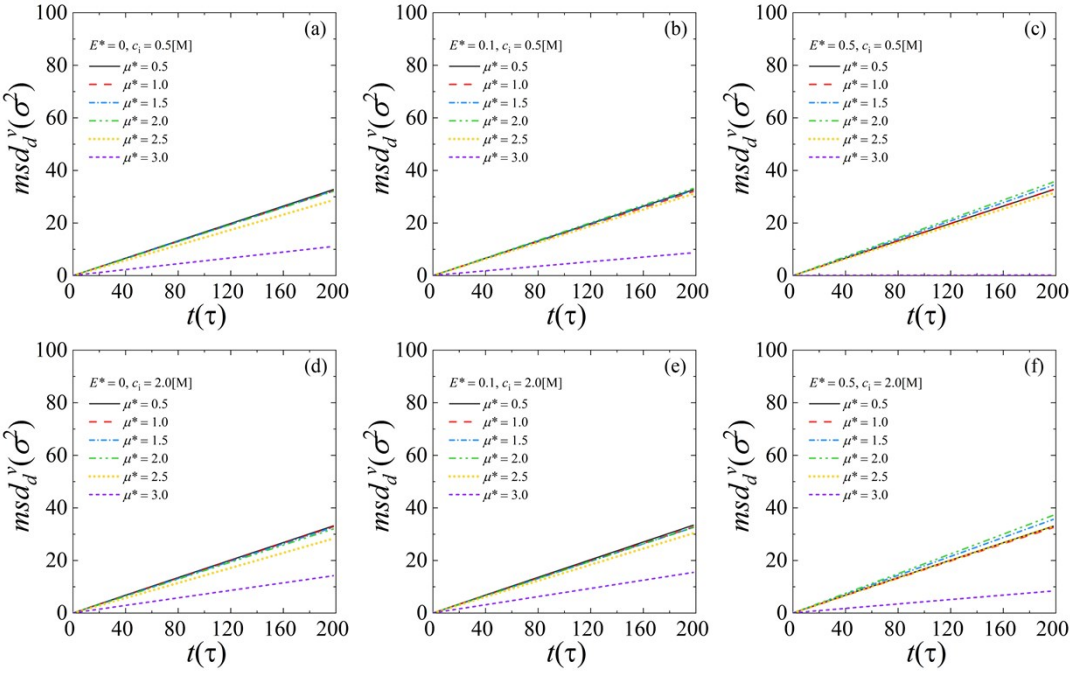

Fig. S8 The components of Mean-squared displacement of dipoles in directions vertical to the electric field as a function of simulation time. The line colors correspond to the values of the dipole moments. (a) c_i =

0.5 [M], E^* = 0, (b) c_i = 0.5 [M], E^* = 0.1, (c) c_i = 0.5 [M], E^* = 0.5, (d) c_i = 2.0 [M], E^* = 0, (e) c_i = 2.0 [M], E^* = 0.1, and (f) c_i = 2.0 [M], E^* = 0.5.