Supplementary material

Preparation and equilibration of the mixtures

The initial configuration is generated by the FCC lattice with a quite low density about 0.2 g/cm^3, by which the overlaps of atoms can be reduced effectively. Then the system is quenched in NVE ensemble for 6 ps to eliminate the big forces, after which the density of the system is increased gradually to a reasonable value (e.g. experimental density) within about 10 ps. To improve the statistical sampling, we simulate the system at 700 K for 50 ps in NpT ensemble. Subsequently, the temperature is reduced to 298 K with an interval of 50 K and 2 ps. Then the system is simulated for 200 ps in NpT ensemble to reach equilibration, and another 200 ps for production. The whole running time is about 480 ps.

To verify whether the running time is enough or not in this work, we performed additional 400 ps simulation for a typical system, i.e. x_1=0.4. Figure A-1 demonstrates the evolution of the system as a function of time. Clearly, the density and total internal energy reach steady values after about 150 ps, and their fluctuations during the production phase (after 280 ps) are small enough. Besides the density and energy, the RDFs with different running times are also compared in Fig. A-2. As is shown, the RDFs between $[bmim]^+$ and N_1 in CH_3CN, with production phases of 200, 400 and 600 ps, are nearly the same.

To verify the system is homogenous, we calculated the average number densities along the three directions, X, Y and Z. In each direction, the box is divided into ten equidistant intervals and the number densities of each species within the intervals are

calculated. Figure A-3 is an example for the production phase of 200 ps. It is shown that the densities along the three directions are the same and the system is homogeneous. The fluctuations of the number density are also small enough for such a relatively small system (less than 256 molecules).

In summary, the running time of 200 ps for production phase is long enough to solve the properties in this work.

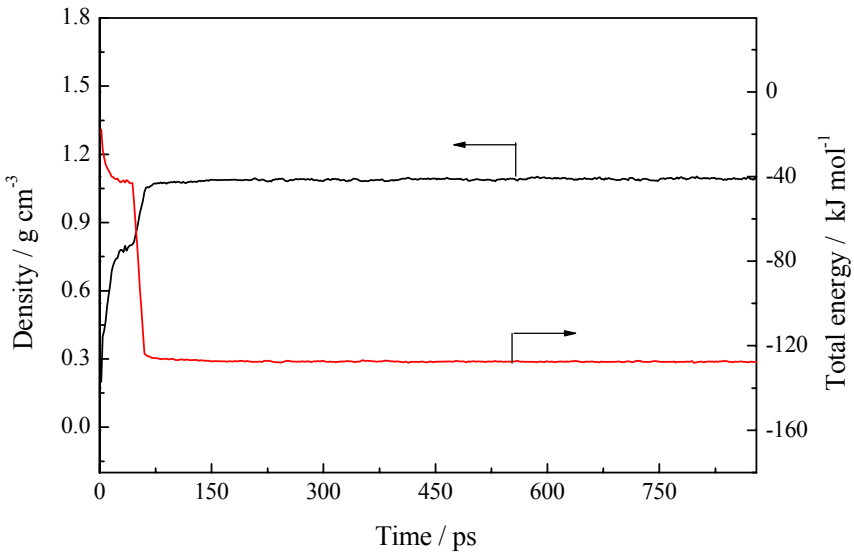

Fig. A-1 Evolution of the system as a function of running time at x_1=0.4

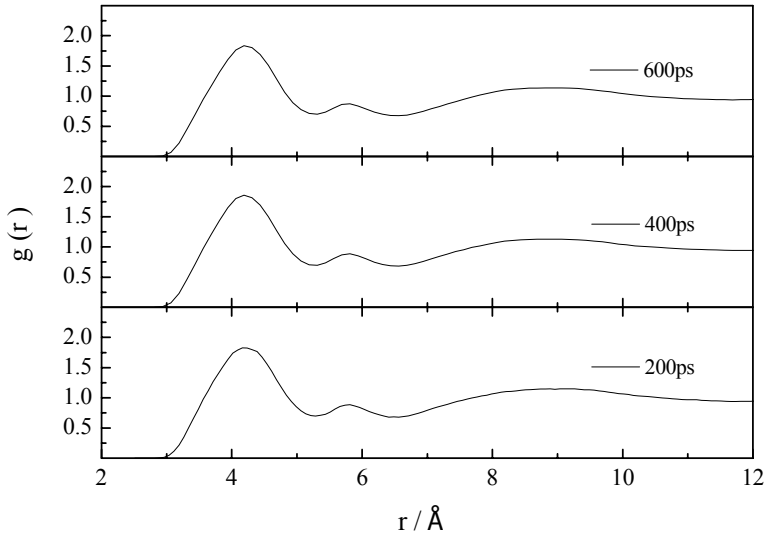

Fig. A-2 RDFs for the centers of the imidazolium ring and the N_1 atoms of CH_3CN at x_1=0.4 with different production phases.

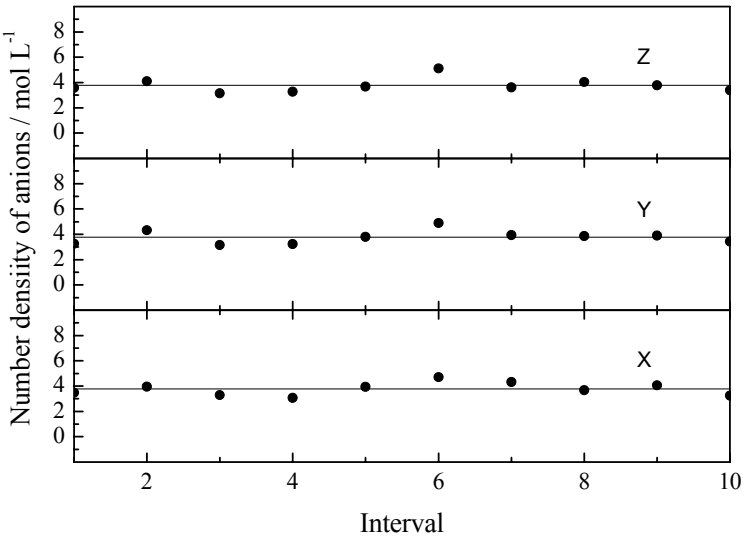

Fig. A-3 Average number densities of anions along three dimensions, X, Y and Z, at x_1=0.4 with the production phase of 200 ps . The lines represent the average number density in the whole box. Dots are those in each interval.