Electronic Supplementary Information (ESI)

Molecular insight into the microstructure and microscopic dynamics of pyridinium ionic liquids with different alkyl chains based on temperature response

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1. The snapshot of polar region and nonpolar region

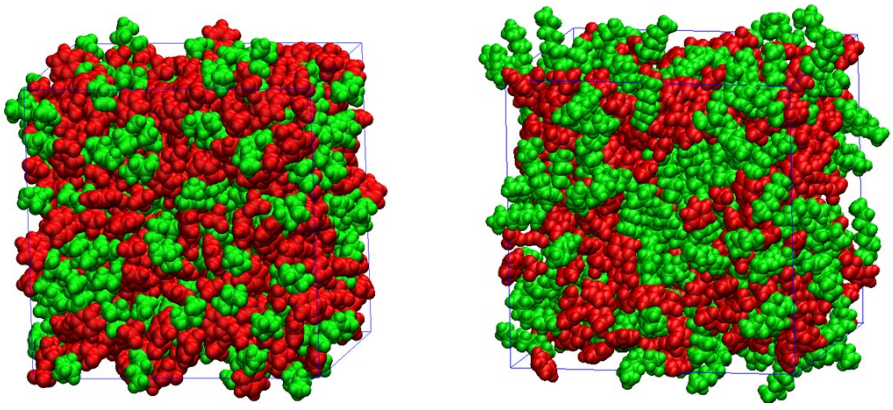

Fig. S1 The snapshot of the polar region and the nonpolar region of [BPy][BF_4] (Left) and [OPy][BF_4] (Right) at 373 K. The polar region was showed in red color including pyridinium ring and anion; the nonpolar region was showed in green color including alkyl chains.

2. The center-of-mass radial distribution functions

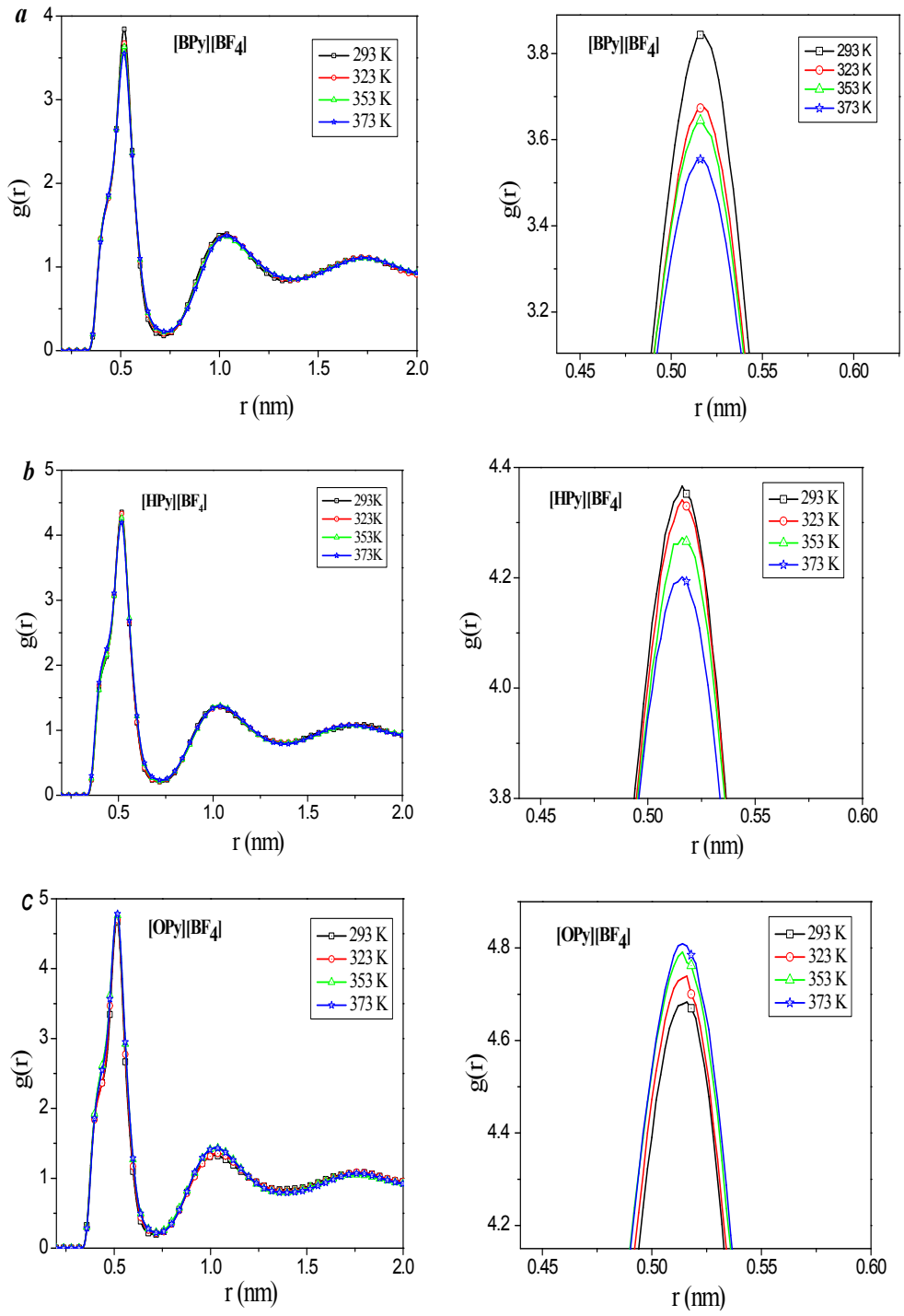

Fig. S2 The center-of-mass RDFs for anions around the pyridine ring of cations. (a). [BPy][BF_4], (b). [HPy][BF_4] and (c). [OPy][BF_4].

3. The spatial distribution functions

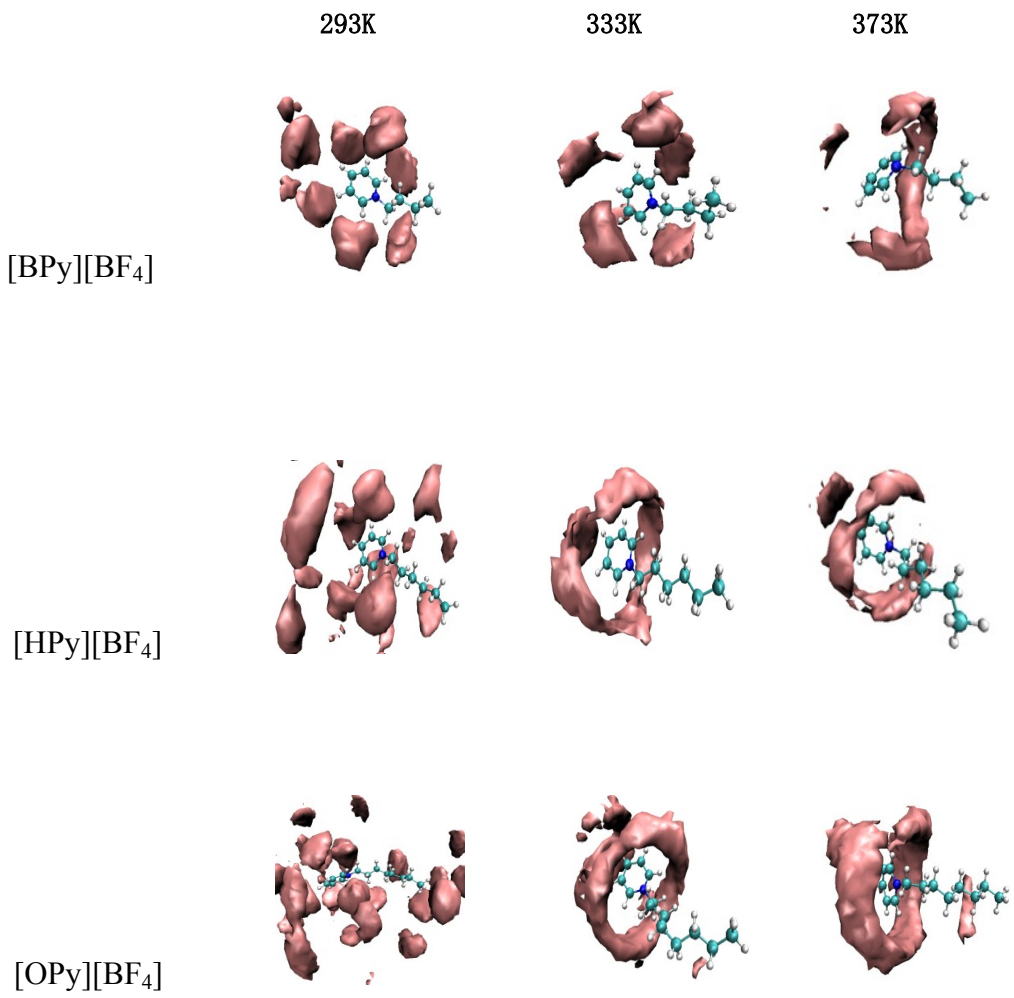

Fig. S3 Spatial distribution of anion around cation, isovalue=22.

4. The velocity autocorrelation functions of cation and anion

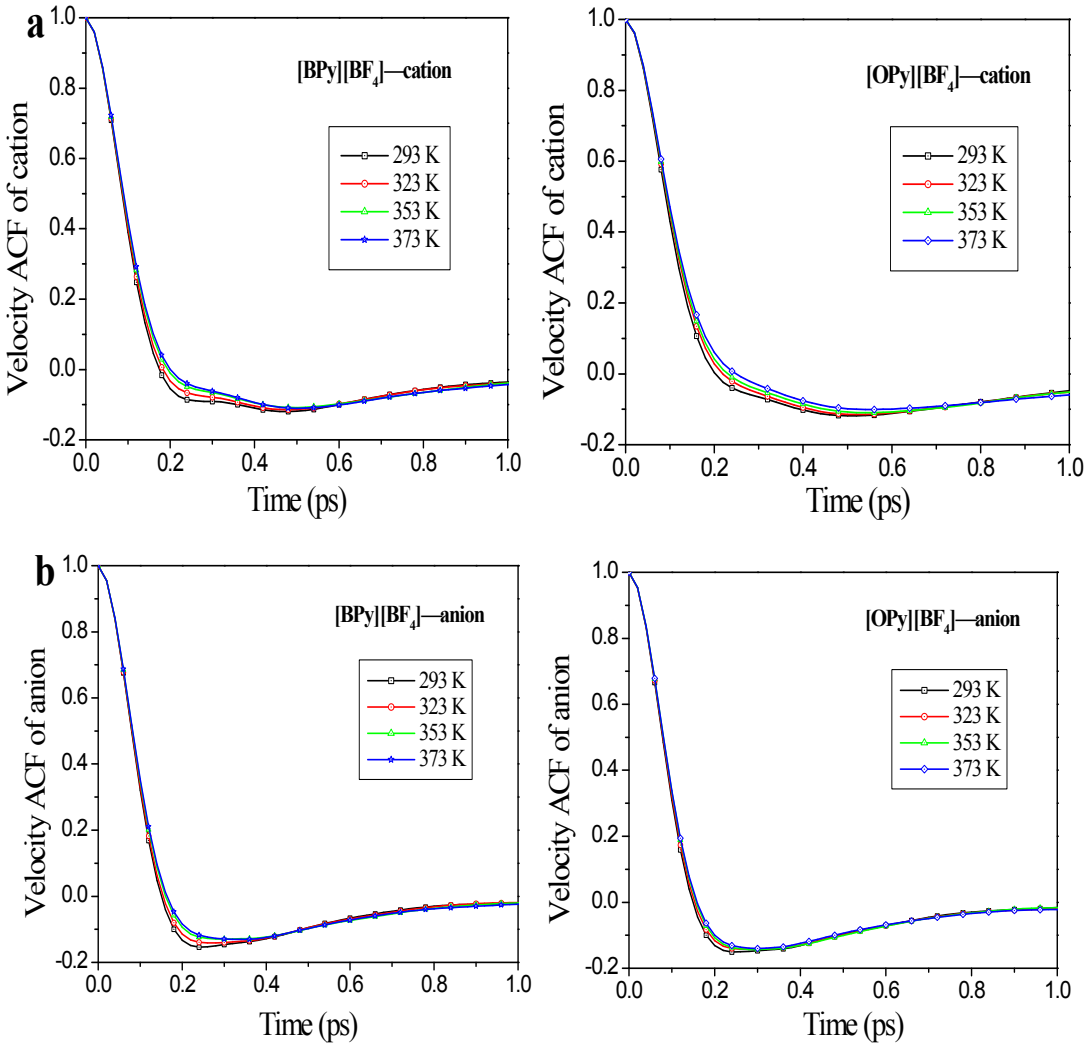

Fig. S4 Velocity autocorrelation functions of cation (a) and anion (b) of $[BPy][BF_4]$ and $[OPy][BF_4]$ under different temperature.

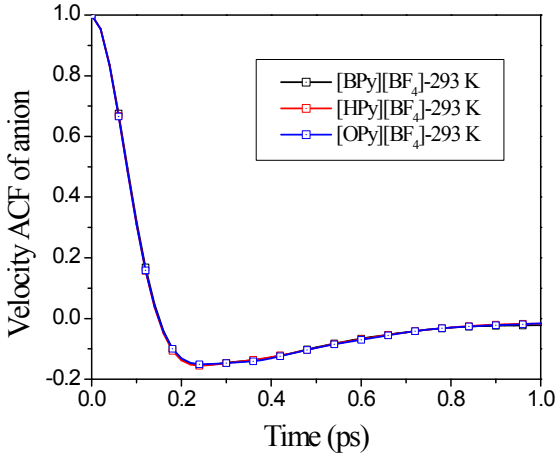

Fig. S5 Velocity autocorrelation functions of anion of three ILs at 293 K.

5. The association dynamics

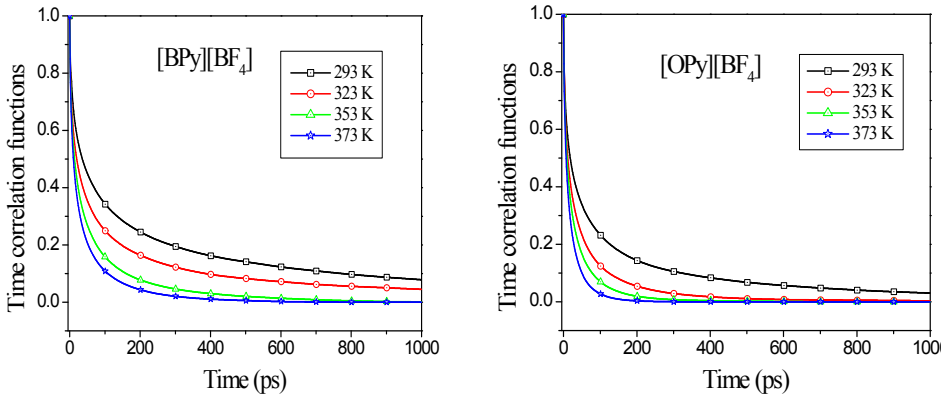

Fig. S6 Time correlation functions of atoms HA1-B under different temperatures.

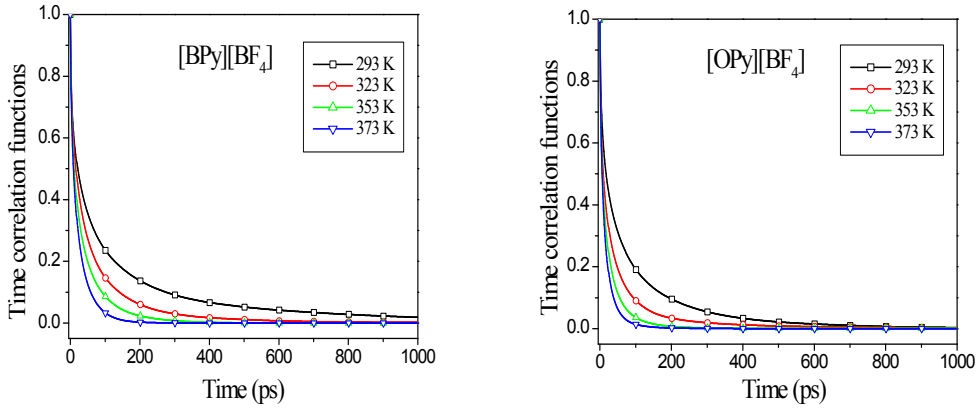

Fig. S7 Time correlation functions of atoms CTn-CTn (n=4, 8) under different temperatures

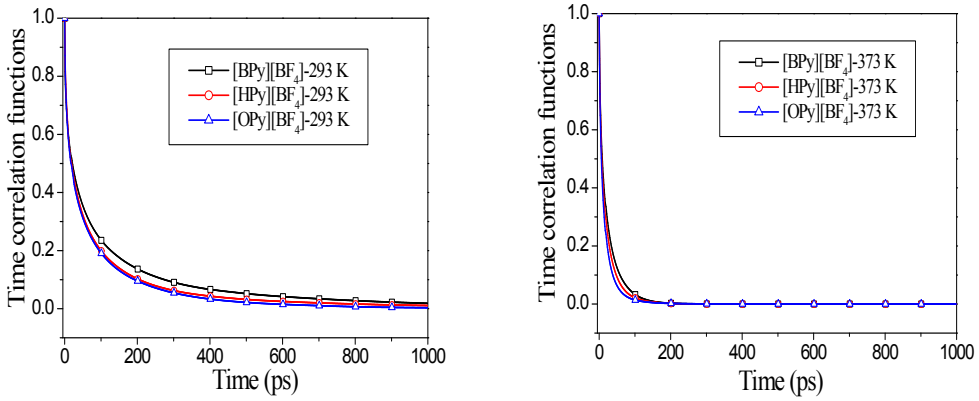

Fig. S8 Time correlation functions of CTn-CTn at 293 K (a) and 373 K (b) of three ILs.