Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Investigation of thermodynamics, structural, dynamical, and electric properties of polyoxometalate ionic liquid into carbon nanotube during the melting process using molecular dynamics simulation

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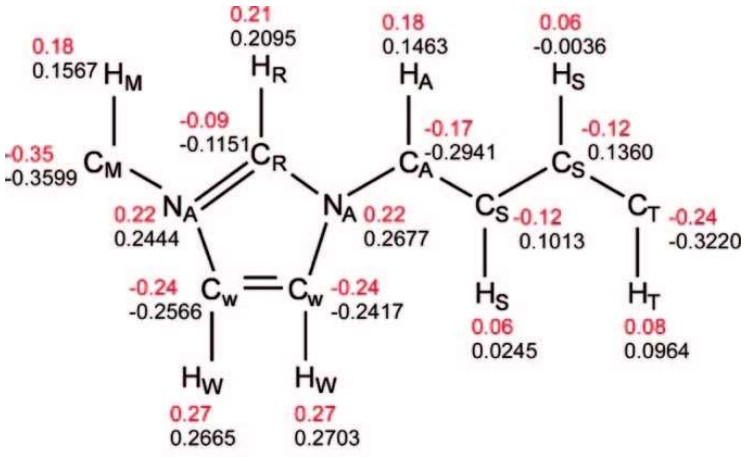
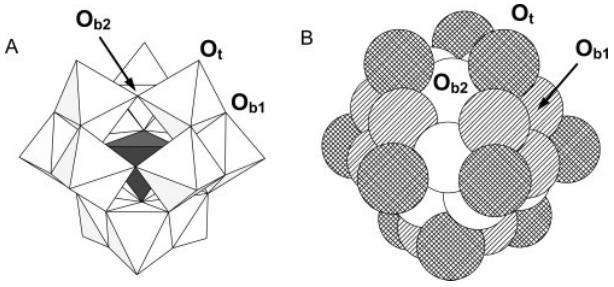
Table S1. The LJ parameters of the cation and anion of the polyoxometallate IL and the CNT used in this work

	ε (kcal/mol)	σ (Å)
P	0.2455	3
W	0.221292	2.34
Ob1	0.214713	3.17
O1	0.214713	3.17
Ob2	0.214713	3.17
CR	0.07	3.55
NA	0.17	3.25
HW=HR	0.03	2.42
CM	0.066	3.5
HM=HA=HT=HS	0.03	2.5
CW	0.066	3.5
C (CNT)	0.055667	3.4





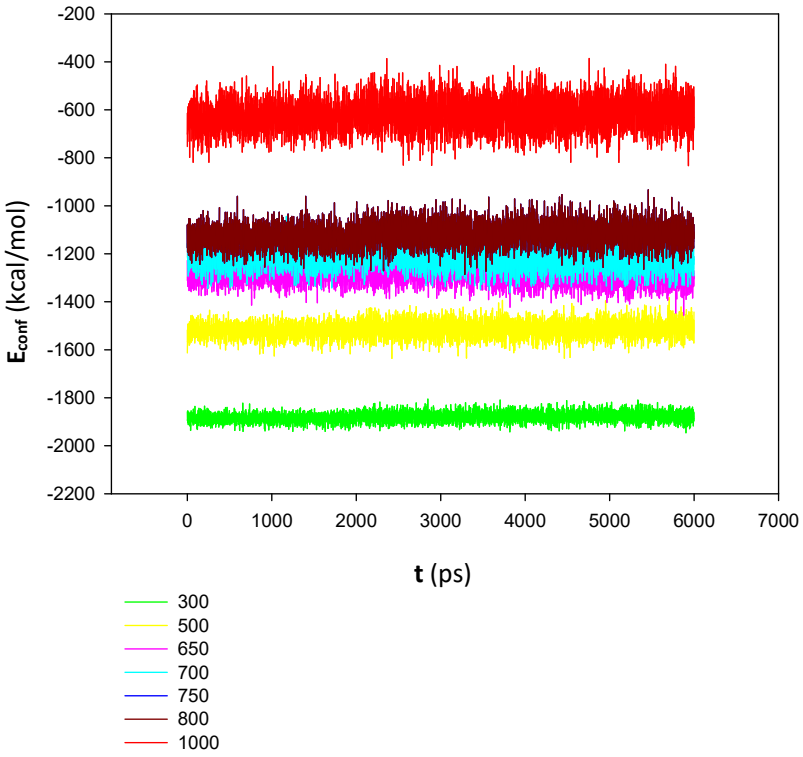


Fig. S1. The configurational energies of the system versus simulation times at different temperatures.

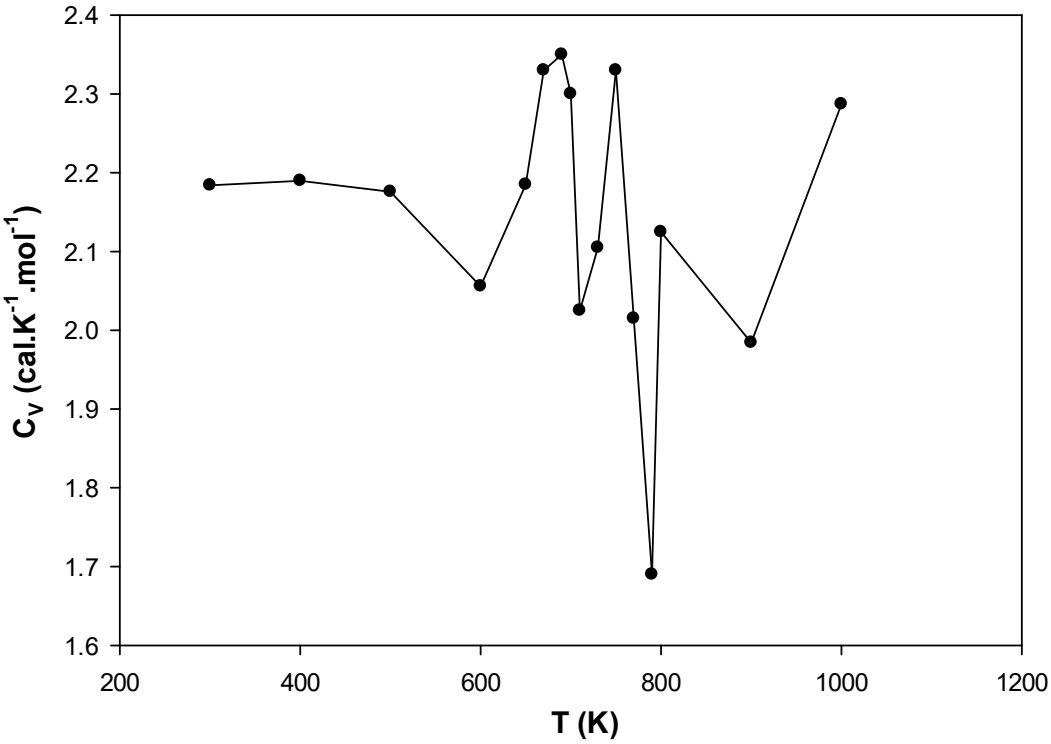


Fig. S2. The heat capacity at constant volume of $[emim]_3[Keggin]$ IL confined into the CNT at different temperatures during the cooling process.

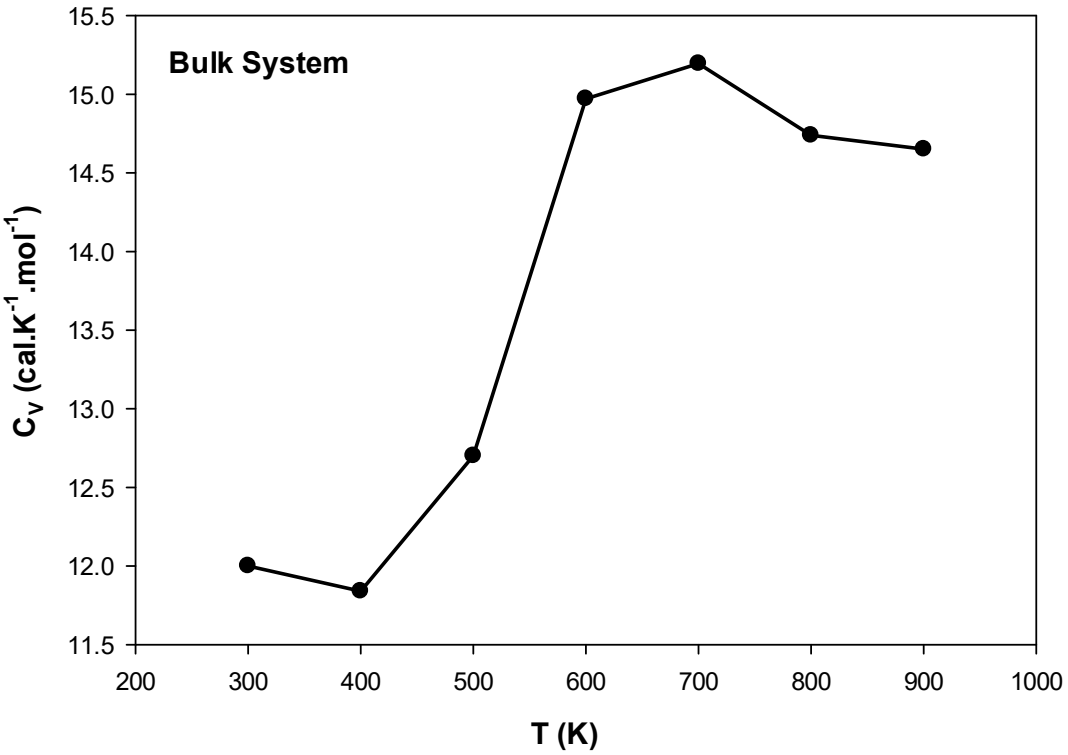


Fig. S3. The heat capacity at constant volume of bulk $[emim]_3[Keggin]$ IL at different temperatures.

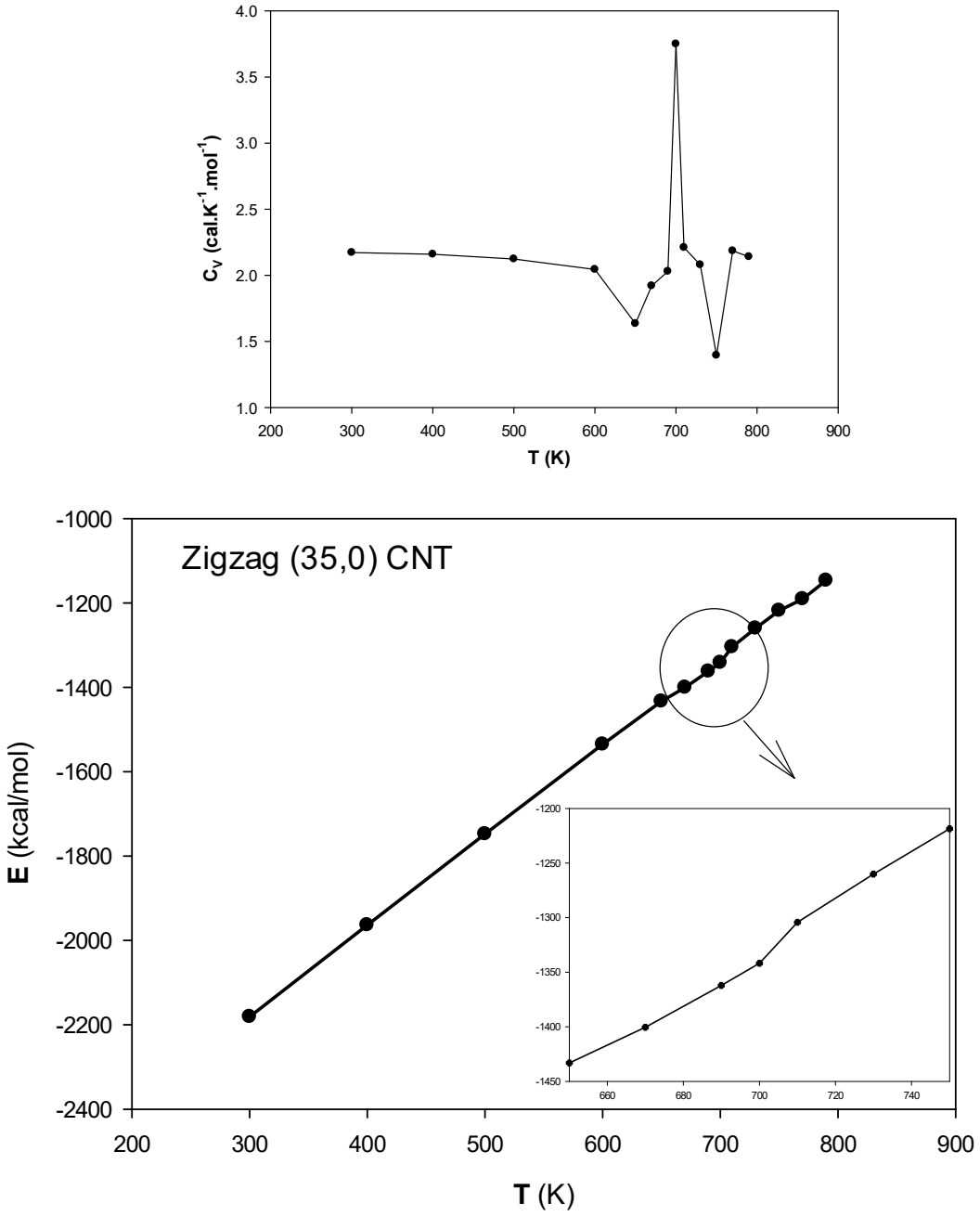


Fig. S4. The configurational energy and heat capacity at constant volume of $[emim]_3[Keggin]$ IL confined in the zigzag (35,0) CNT at different temperatures.

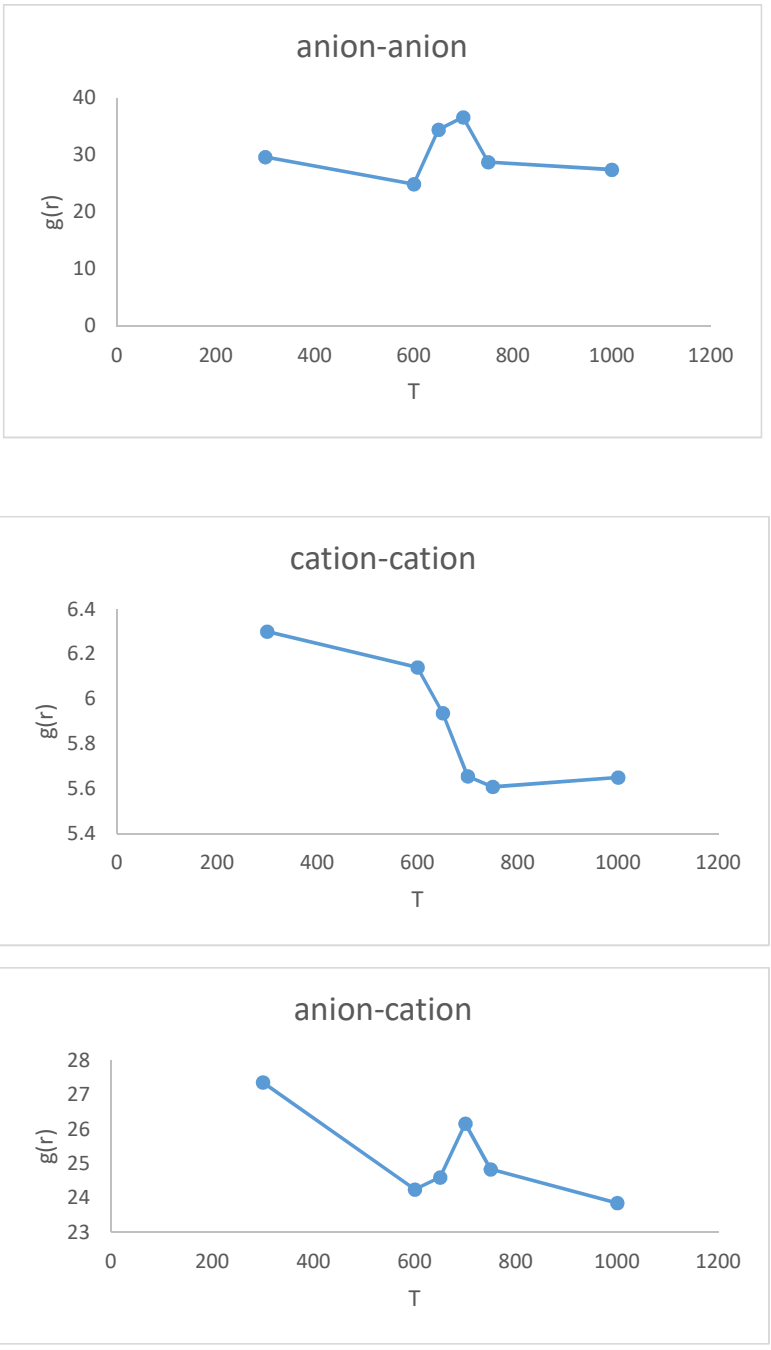


Fig. S5. The maximum points of the first RDF peaks at the different temperatures.

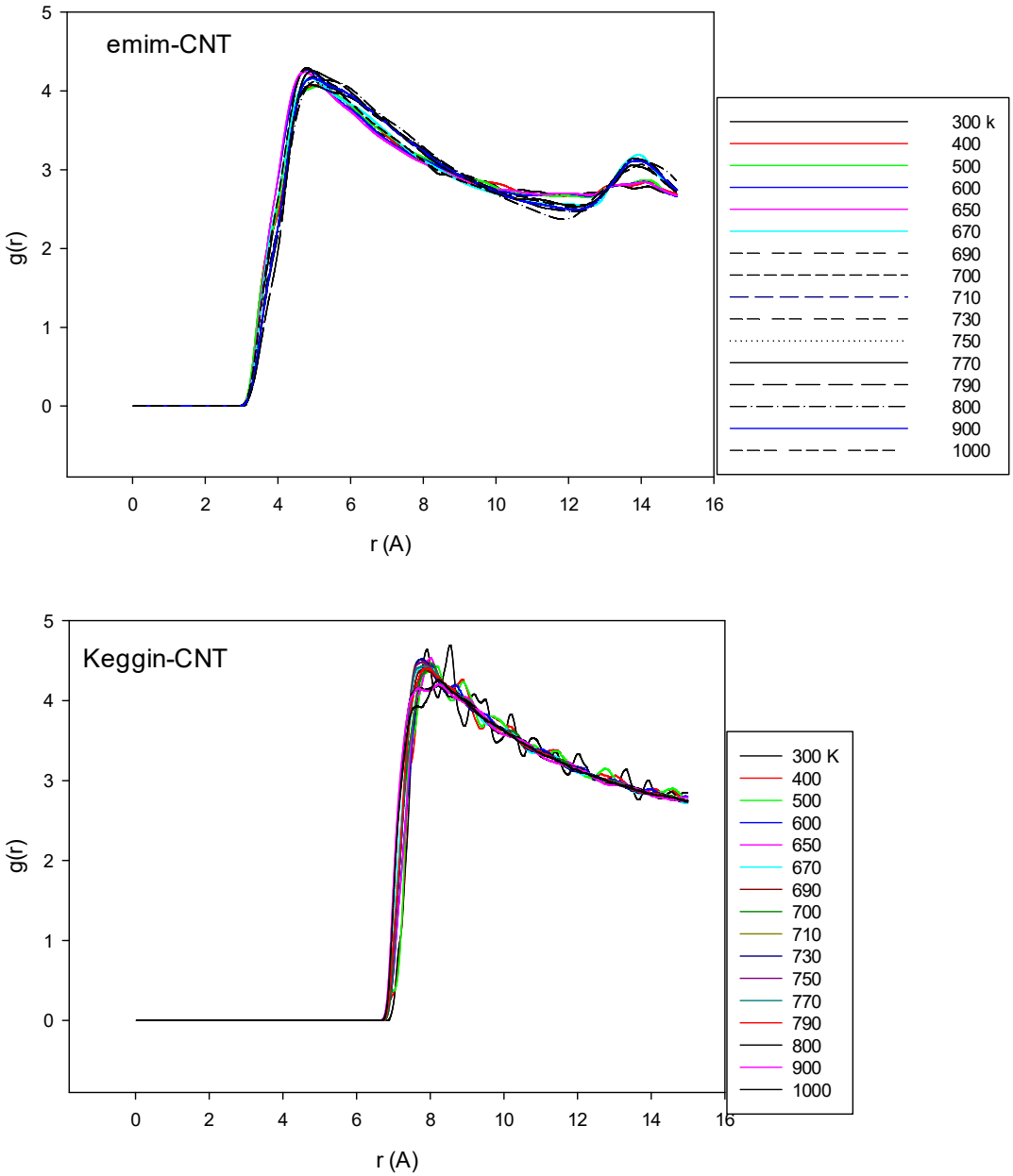


Fig. S6. The cation-CNT and anion-CNT RDFs of $[emim]_3[Keggin]$ system at different temperatures. The nitrogen atom has been selected as the representative of the cation and the phosphorus atom has been chosen in the case of the anion.

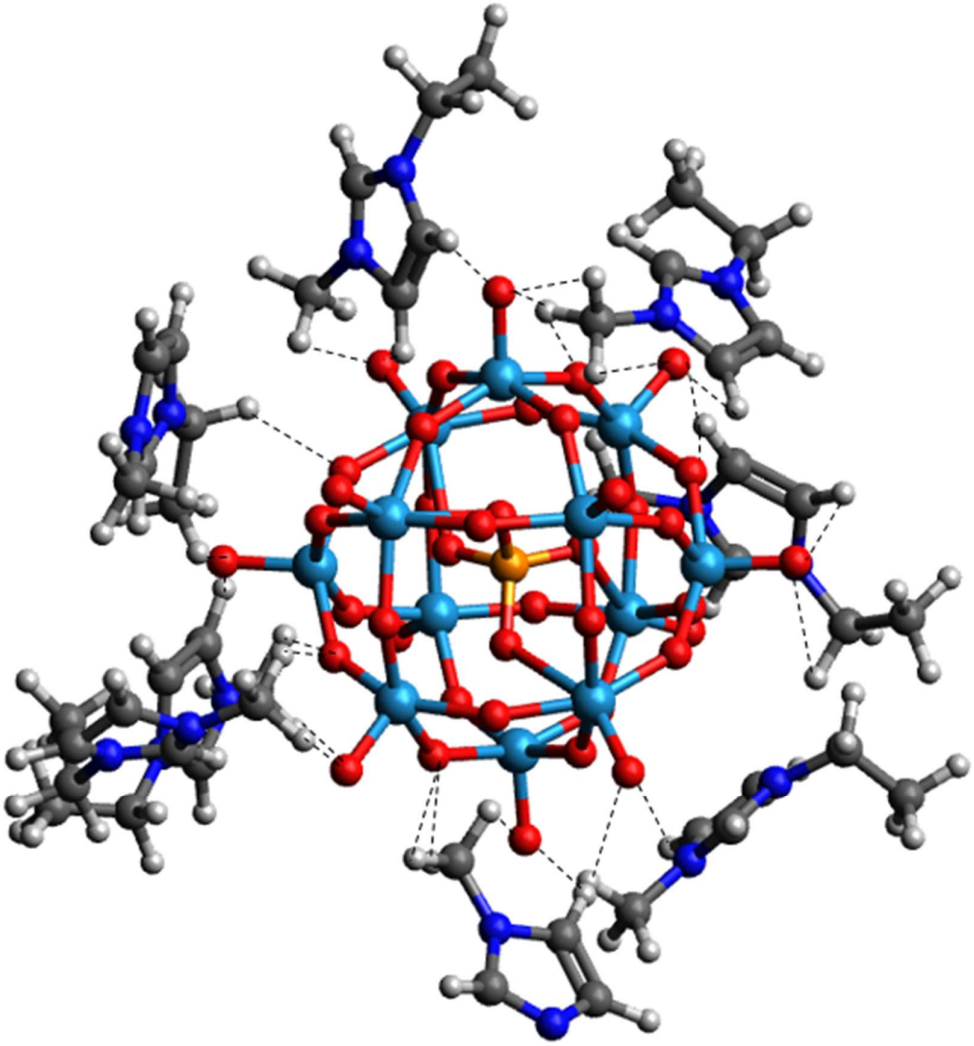


Fig S7. The HBs between H atoms from emim cations and O atoms from Keggin anion (according to the final configuration of the confined IL in CNT at 500 K). We consider the criteria for HB that if the distance between the hydrogen atom in cation and oxygen atom in anion is less than 2.67 Å, then the interaction can be recognized as HB[27,41]

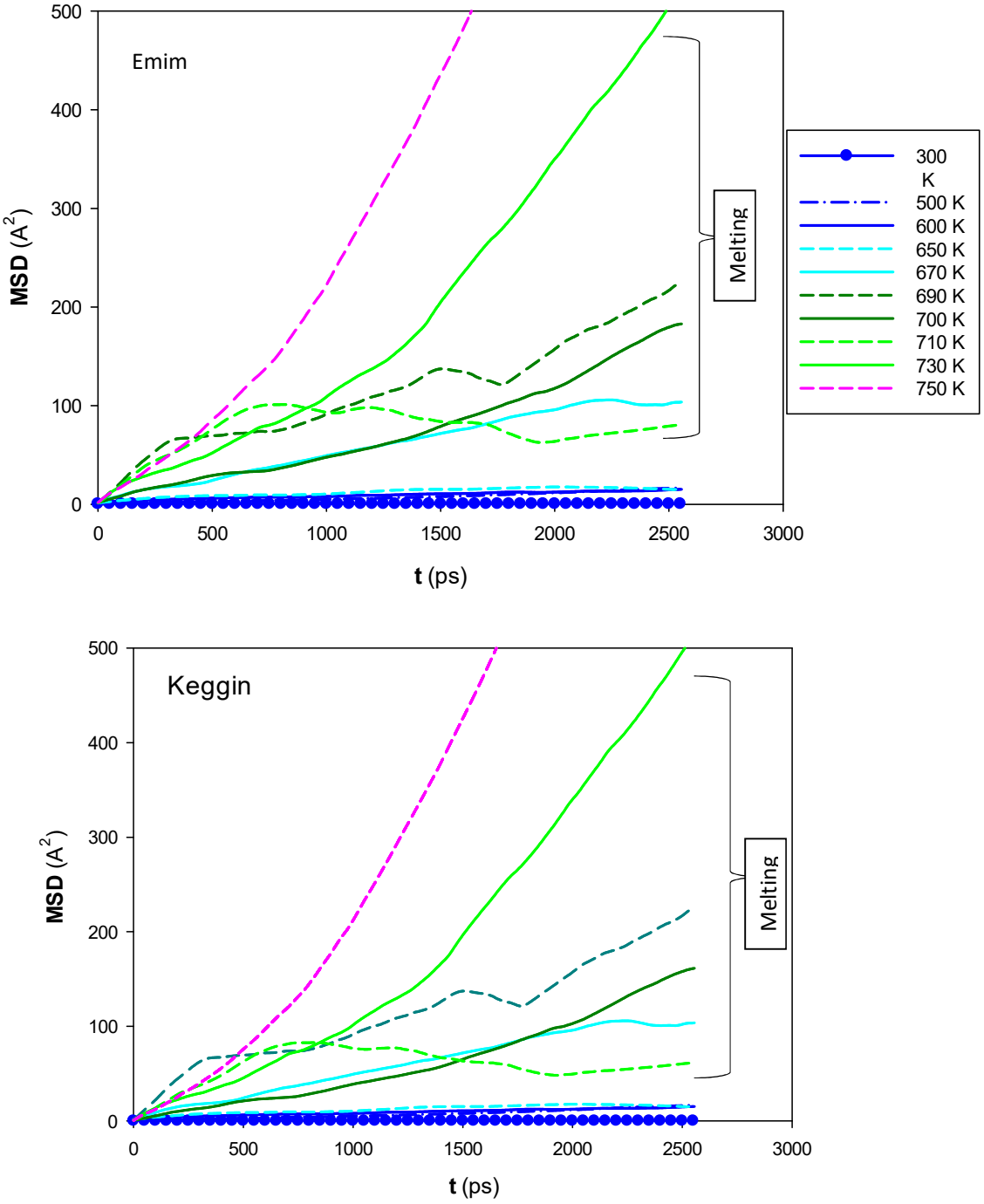


Fig. S8. The MSD of cation and anion versus simulation times at the different temperatures.