Electronic Supplementary Material (ESI) for RSC Advances.

Effect of Interionic interactions on the Structure and Dynamics of Ionic Solvation Shell in Aqueous Electrolyte Solutions

Parveen Kumar[*,a]*, Mridula Dixit Bharadwaj*[a] *and S. Yashonath*[b]

[a]*Center for Study of Science, Technology and Policy, Bangalore-560094, India*

[b]*Solid Sate and Structural Chemistry Unit, Indian Institute of Science, Bangalore-560012, India*

E-mail : parveen@cstep.in; kparveen79@gmail.com

Figure S1 : For 0.05 M LiF electrolyte solution, the initial configuration was equilibrated for 500 ps, and the last configuration was taken as starting configuration for the final simulation run which includes 500 ps of equilibration followed by 5 ns of production run. The average temperature lies between 293-301 K, with RMS fluctuations of 1.6 K.

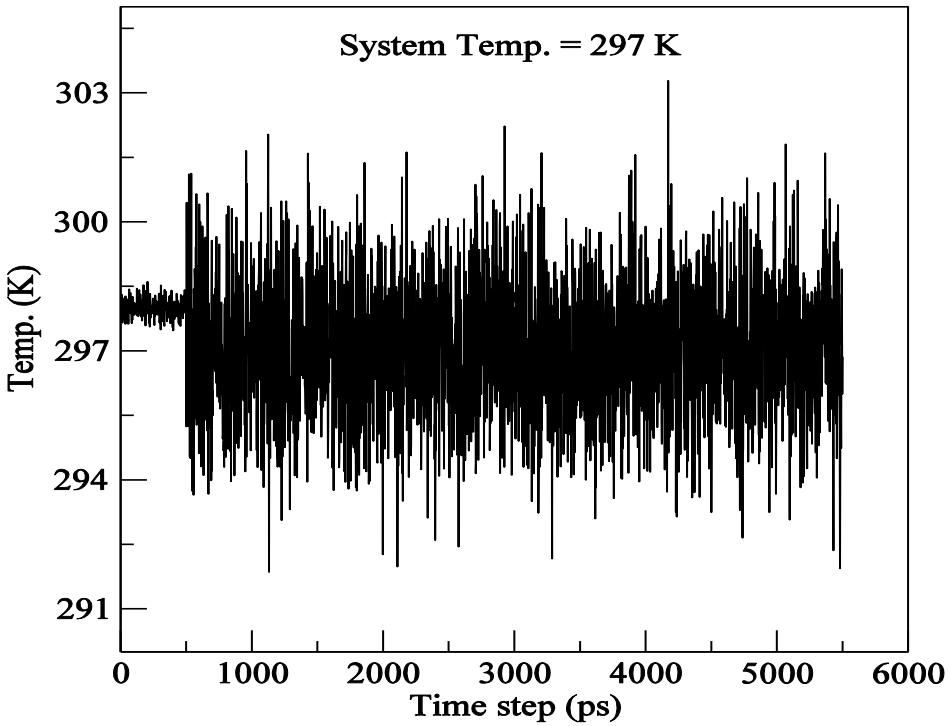

Figure S2 : Effect of simulation run length and system size on the trend in RDF plots for (a) F^--O and (b) Li^+-O for LiF in SPC/E water at 298 K. Here, small system consist of 8 LiF in 848 SPC/E water molecules and big system consist of 75 LiF in 8042 SPC/E water.