Supplementary Material

Revised Atomic Charges for OPLS Force Field Model of Poly(Ethylene Oxide): Benchmarks and Applications in Polymer Electrolyte

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1. Simulation system list

Table S1. Pure PEO systems

	OPLS	**BARBOSA**	**RESP**
Different T	20ns for each T	20ns for each T	20ns for each T
298K equilibrium	150ns	400ns	700ns

Table S2. Electrolyte system ([EO]/[Li^+] =16)

	OPLS	**RESP(1/1)**	**RESP(0.8/0.55)**
298K	300ns	300ns	200ns
333K	300ns	300ns	200ns
363K	300ns	300ns	500ns

Table S3. Electrolyte system ($OPLS^R$ force field with different [EO]/[Li^+] ratio at 363K)

System([EO]/[Li^+])	***Simulation time***
16 (0.8/0.55)	500ns
25 (0.8/0.55)	500ns
50 (0.8/0.55)	500ns

2. Diffusion of TFSI (333K, [EO]/[Li^+]=16)

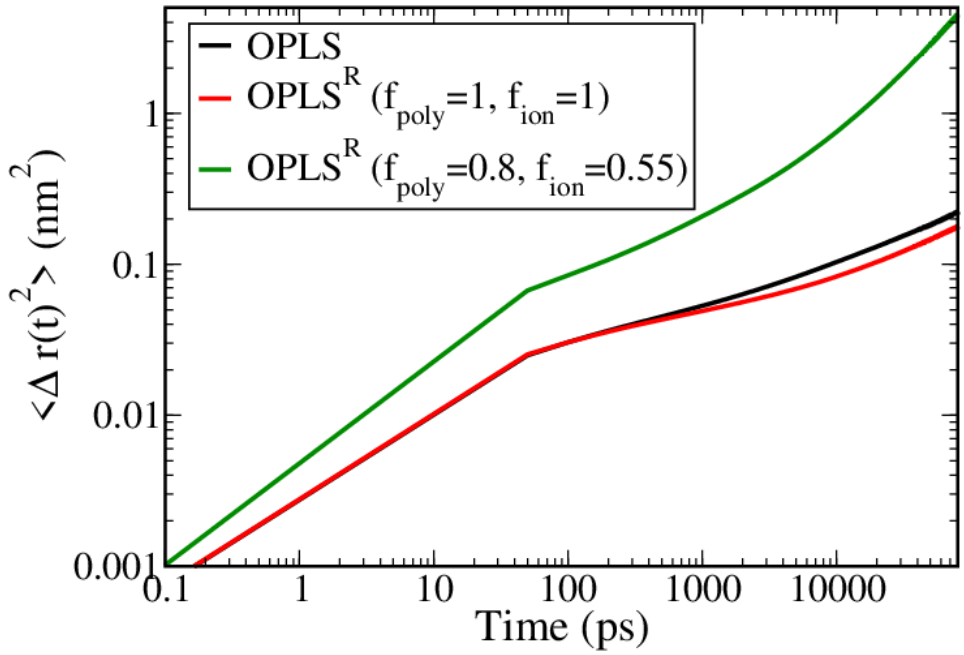

Figure s1. The mean square displacement profiles of TFSI in PEO/LiTFSI SPE system at 333K for three tested force fields.

3. Diffusion of Li^+ at different temperature ([EO]/[Li^+]=16)

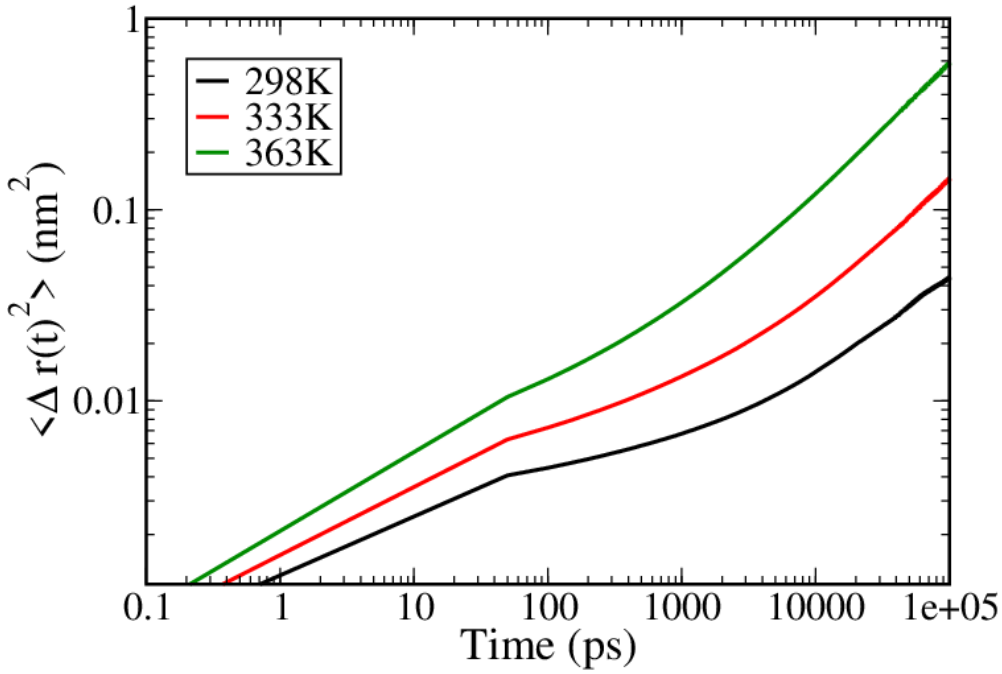

Figure s2. The mean square displacement profiles of Li^+ in PEO/LiTFSI SPE system at different temperature of default OPLS force field.

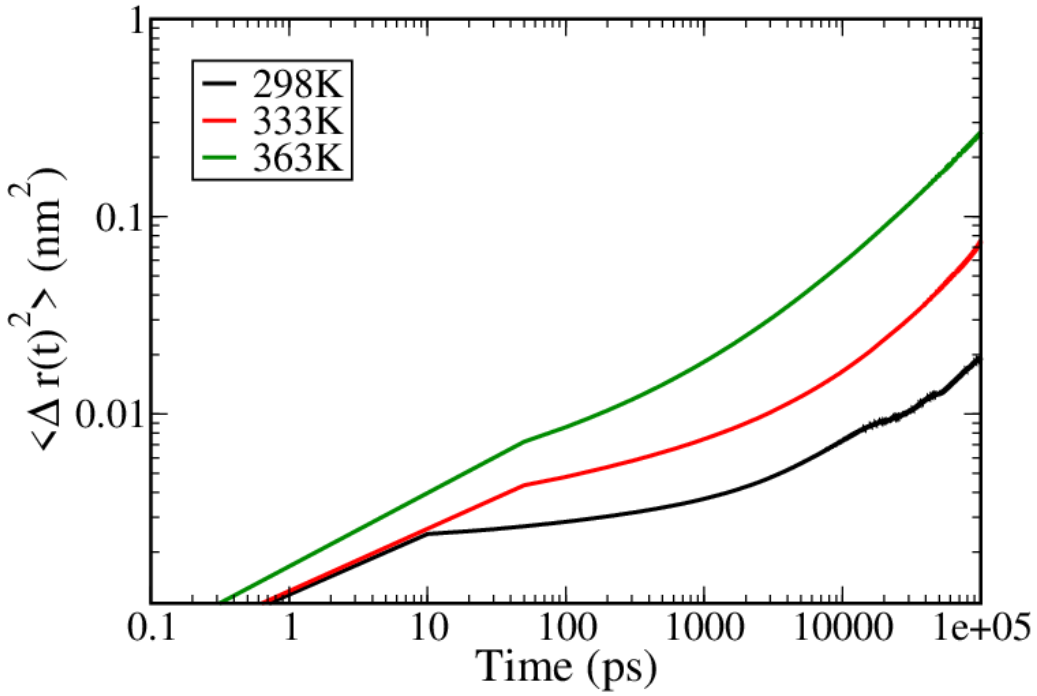

Figure s3. The mean square displacement profiles of Li^+ in PEO/LiTFSI SPE system at different temperature of OPLS^R force field with scaling factor (f_{poly} = 1, f_{ion} = 1).

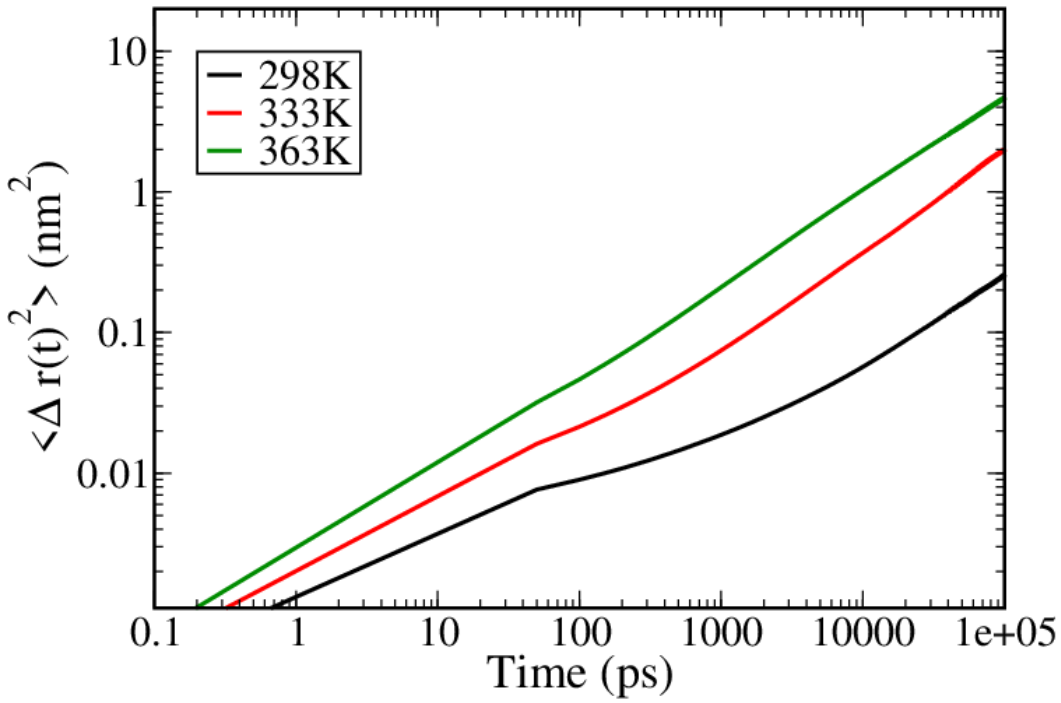

Figure s4. The mean square displacement profiles of Li^+ in PEO/LiTFSI SPE system at different temperature of OPLS^R force field with scaling factor (f_{poly} = 0.8, f_{ion} = 0.55).

4. Diffusion of TFSI at different temperature ([EO]/[Li^+]=16)

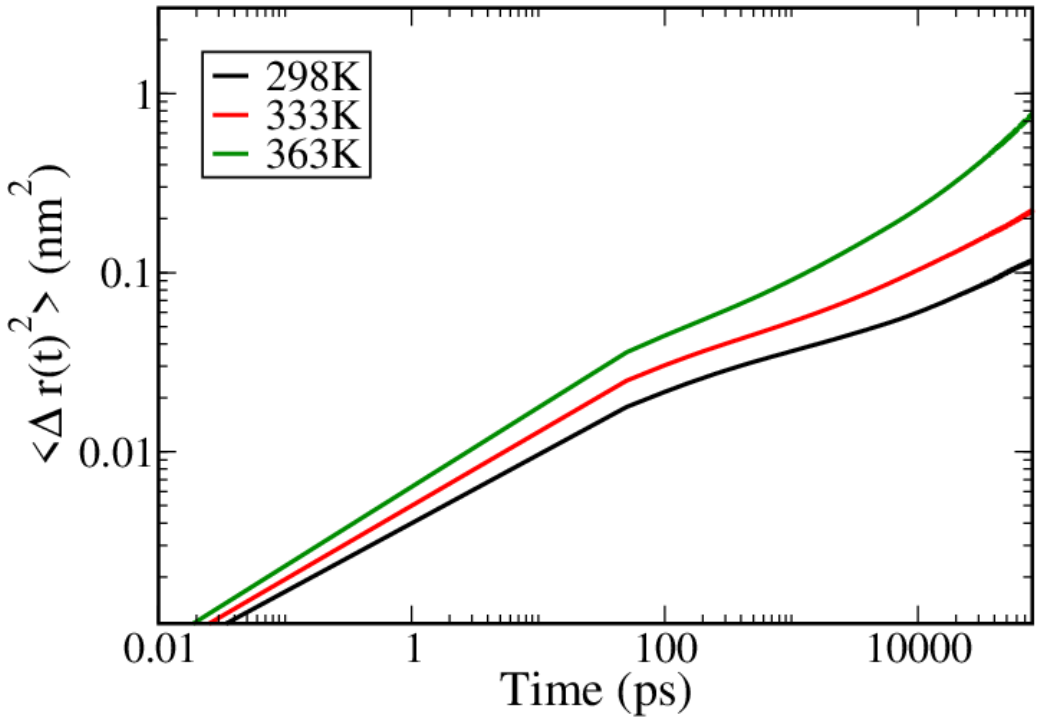

Figure s5. The mean square displacement profiles of TFSI in PEO/LiTFSI SPE system at different temperature of default OPLS force field.

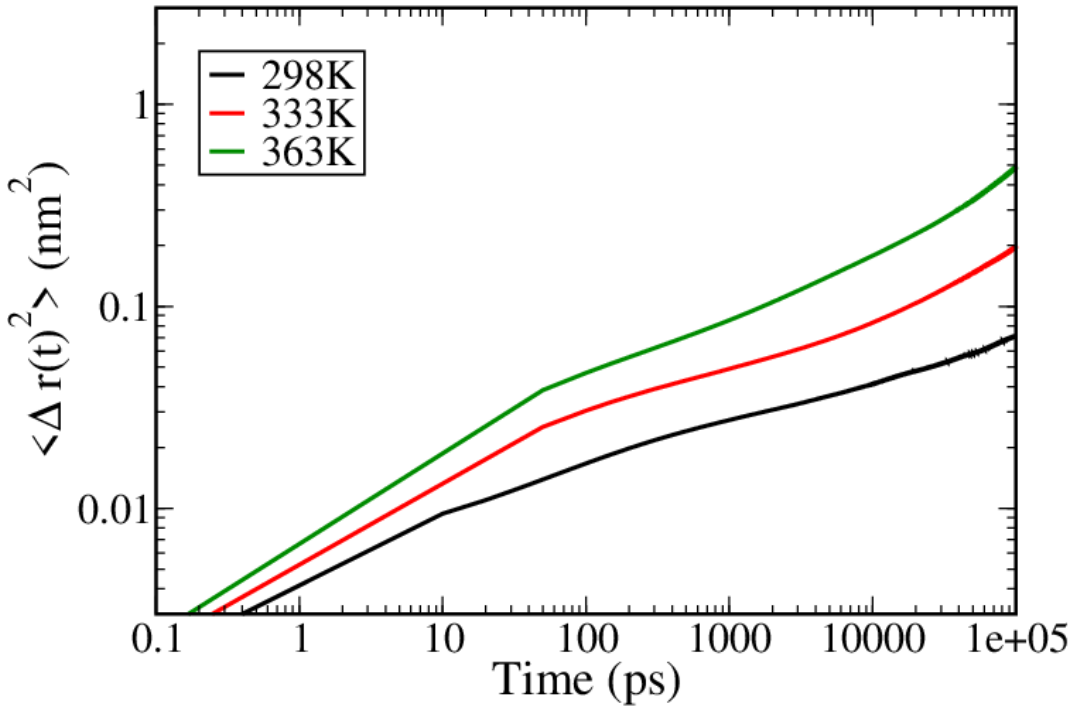

Figure s6. The mean square displacement profiles of TFSI in PEO/LiTFSI SPE system at different temperature of $OPLS^R$ force field with scaling factor (f_{poly} = 1, f_{ion} = 1).

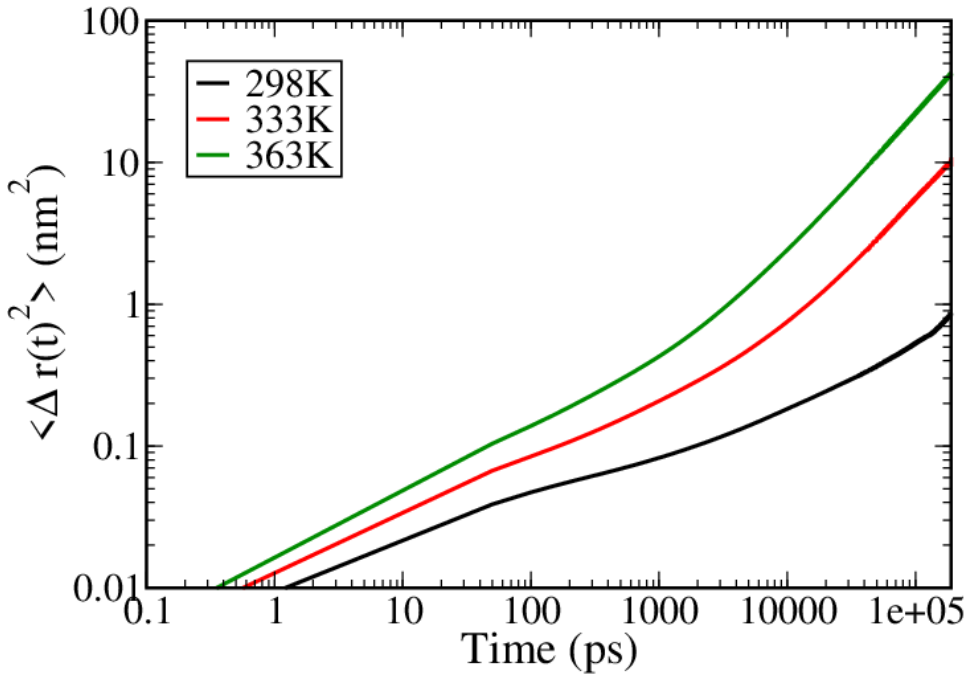

Figure s7. The mean square displacement profiles of TFSI in PEO/LiTFSI SPE system at different temperature of OPLS^R force field with scaling factor (f_{poly} = 0.8, f_{ion} = 0.55).

5. Diffusion of Li^+ in different [EO]/[Li^+] ratio at 363K

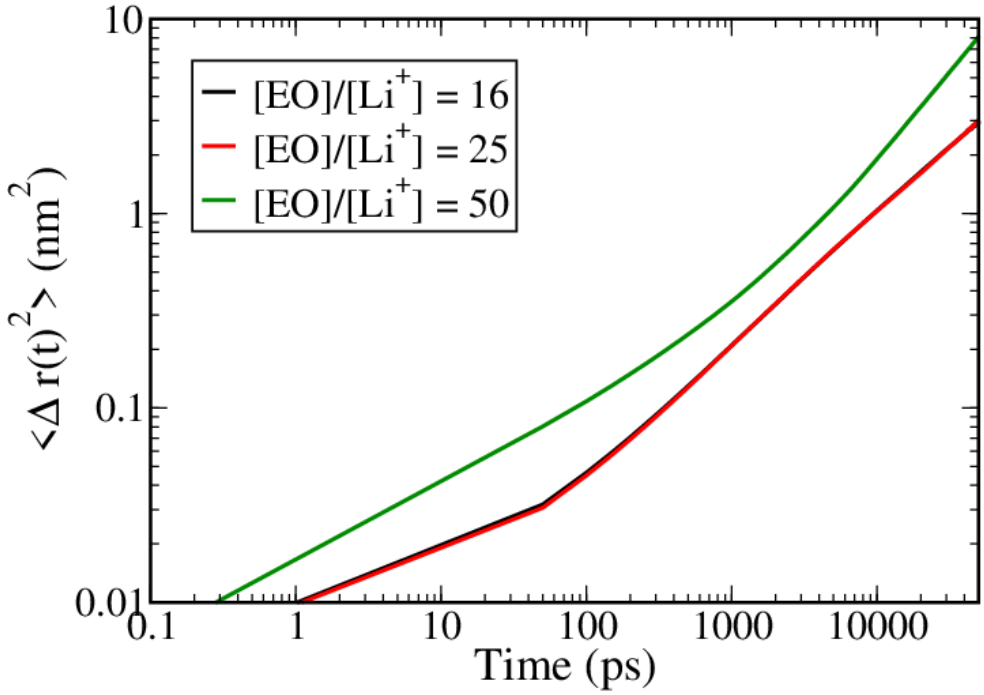

Figure s8. The mean square displacement profiles of Li^+ in PEO/LiTFSI SPE system at [EO]/[Li^+] ratio of OPLS^R force field with scaling factor (f_{poly} = 0.8, f_{ion} = 0.55).