Supporting Information for

Interplay Between Organic Solvent Geometry and Divalent Cation Dynamics

*Nazifa Jahan Pranti[1], Sharifa Faraezi[1], Tomonori Ohba[2], Argyrios V. Karatrantos,[3] and Md Sharif Khan[1]**

[1]Center for Interdisciplinary Chemistry Research (CICR). Dhaka, Bangladesh

[2]Graduate School of Science, Chiba University, 1-33 Yayoi, Inage, Chiba 263-8522,Japan

[3]Luxemburg Institute of Science and Technology, 5, avenue des Hauts-Fourneaux,

L-4362 Esch-sur-Alzette, Luxembourg

Corresponding Author

* E-mail: sharifkhanjnu@gmail.com

Figures S1 –S5

	Atom Type	Sigma (nm)	Epsilon (kj / mol)
EC	OE	2.96000e-01	8.7864000e-01
	CE	3.75000e-01	4.393200e-01
	OSE	3.00000e-01	7.11280e-01
	C1E	3.50000e-01	2.7614400e-01
	C2E	3.50000e-01	2.7614400e-01
	H2E	2.42000e-01	6.276100e-02
	H1E	2.42000e-01	6.276100e-02
PC	OP	2.96000e-01	8.7864000e-01
	CP	3.75000e-01	4.393200e-01
	OAP	3.00000e-01	7.11280e-01
	C2P	3.50000e-01	2.7614400e-01
	C1P	3.50000e-01	2.7614400e-01
	OBP	3.00000e-01	7.11280e-01
	C3P	3.50000e-01	2.7614400e-01
	H1P	2.4200e-01	6.276000e-02
	H2P	2.42000e-01	6.276000e-02
	H3P	2.42000e-01	6.276000e-02
EMC	C1M	3.75000e-01	4.393200e-01
	O1M	3.00000e-01	7.11280e-01
	O2M	3.00000e-01	7.11280e-01
	O3M	2.96000e-01	8.7864000e-01
	C2M	3.50000e-01	2.7614400e-01
	C3M	3.50000e-01	2.7614400e-01
	C4M	3.50000e-01	2.7614400e-01
	H1M	2.42000e-01	6.276100e-02
	H2M	2.42000e-01	6.276100e-02
	H3M	2.42000e-01	6.276100e-02
	H4M	2.42000e-01	6.276100e-02
	H5M	2.42000e-01	6.276100e-02
	H6M	2.42000e-01	6.276100e-02
	H7M	2.42000e-01	6.276100e-02
	H8M	2.42000e-01	6.276100e-02
TFSI	NJ	3.25000e-01	7.1128e-01
	SJ	3.55000e-01	1.0460e-00
	OJ	2.96000e-01	8.7864e-01
	CJ	3.50000e-01	2.7614e-01
	FJ	2.95000e-01	2.2175e-01
Mg^{2+}	Mg	2.38500e-01	6.2000e-01
Ca^{2+}	Ca	2.70800e-01	12.200e-01

Table S1: Force field parameters of the different solvent and TFSI used in this study

	Solvent Number	Cation Number	Anion Number
EC	1128	37	74
PC	888	37	74
EMC	734	37	74

Table S2: Total number of solvents, cations and anions used in the simulation box

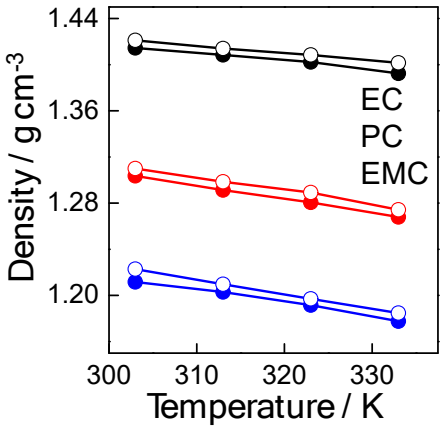

Figure S1: Change of the density of the electrolytes systems of Mg^{2+} (closed circle) and Ca^{2+} (open circle) as a function of temperature

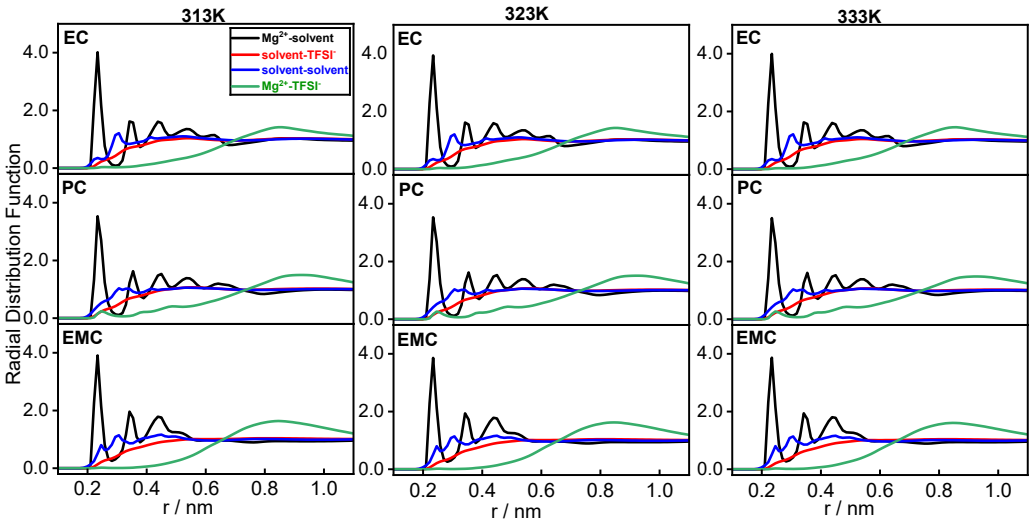

Figure S2: Radial distribution function of the different correlations Mg^{2+} - solvent (black), solvent – solvent (Blue), $TFSI^-$ - solvent (red), and Mg^{2+} - $TFSI^-$ (green) in different solvents at 313, 323 and 333 K temperatures.

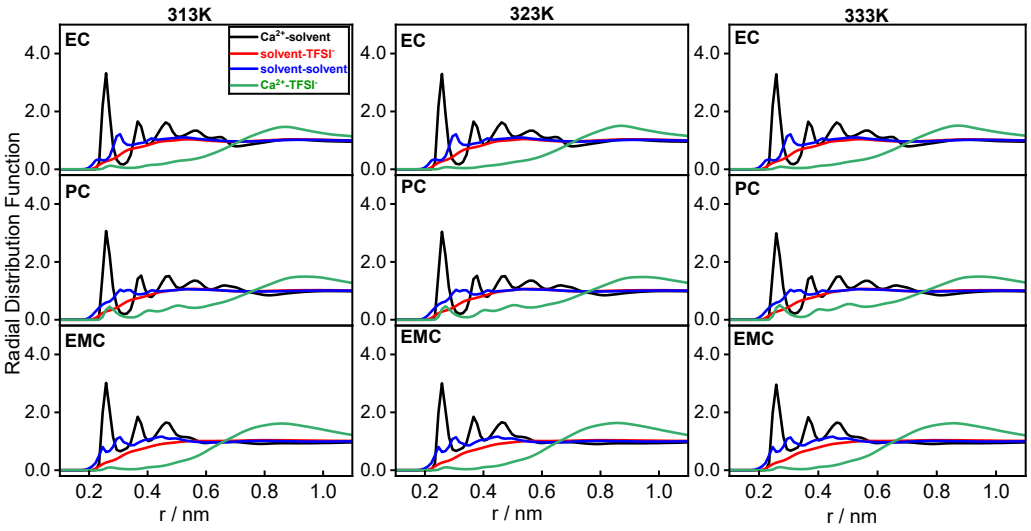

Figure S3: Radial distribution function of the different correlations Ca^{2+} - solvent (black), solvent – solvent (Blue), $TFSI^-$ - solvent (red), and Ca^{2+} - $TFSI^-$ (green) in different solvents at 313, 323 and 333 K temperatures.

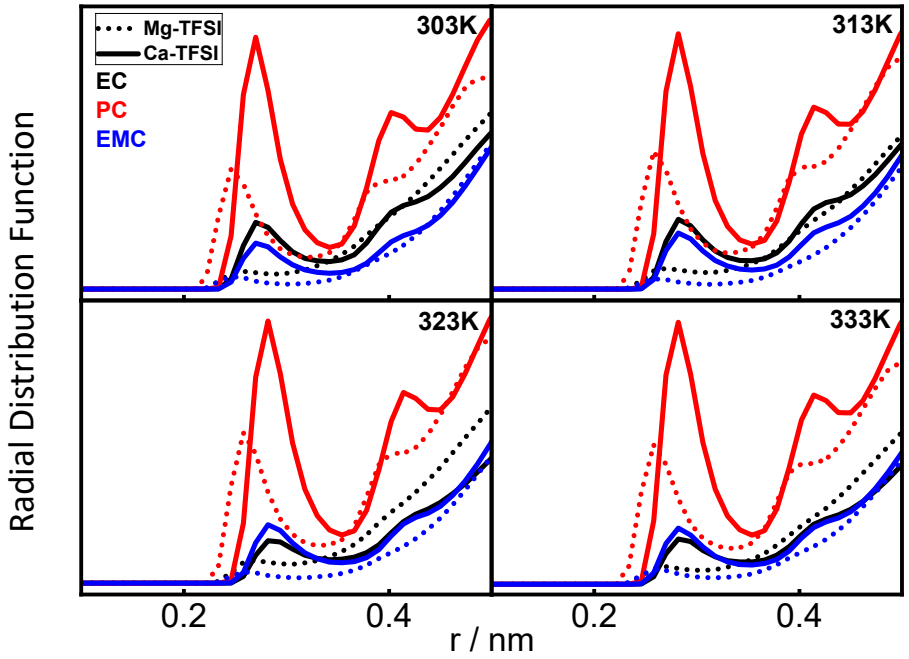

Figure S4: Radial distribution function between the Mg^{2+} - $TFSI^-$ and Ca^{2+} - $TFSI^-$ in different solvents at different applied temperatures.

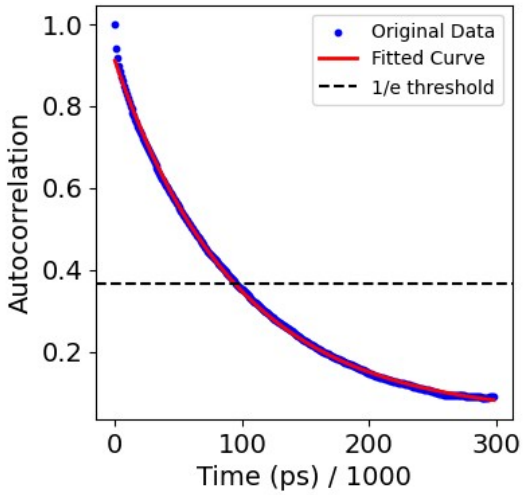

Figure S5: Example fit for the autocorrelation of the residence time to the equation of 4 of the main manuscript, here it is for Mg^{2+} ion in PC solvent.