

# Theoretical insights into the dissolution of LiFSI in weakly and strongly solvating solvents

Maipelo Nyepetsi<sup>a</sup>, Foster Mbaiwa<sup>\*a</sup>

Supporting information

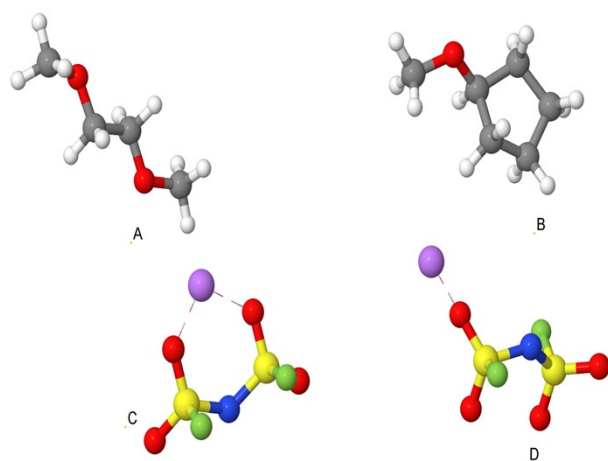


Figure S1: Geometrical structures of the solvents investigated in this DME (A), CPME (B) and the FSI anion and its interaction mode with Li<sup>+</sup> (C and D)

\* Corresponding Author

<sup>a</sup> Department of Chemical and Forensic Sciences, Botswana International University of Science and Technology, Palapye, Botswana

Email: [mbaiwaf@biust.ac.bw](mailto:mbaiwaf@biust.ac.bw)

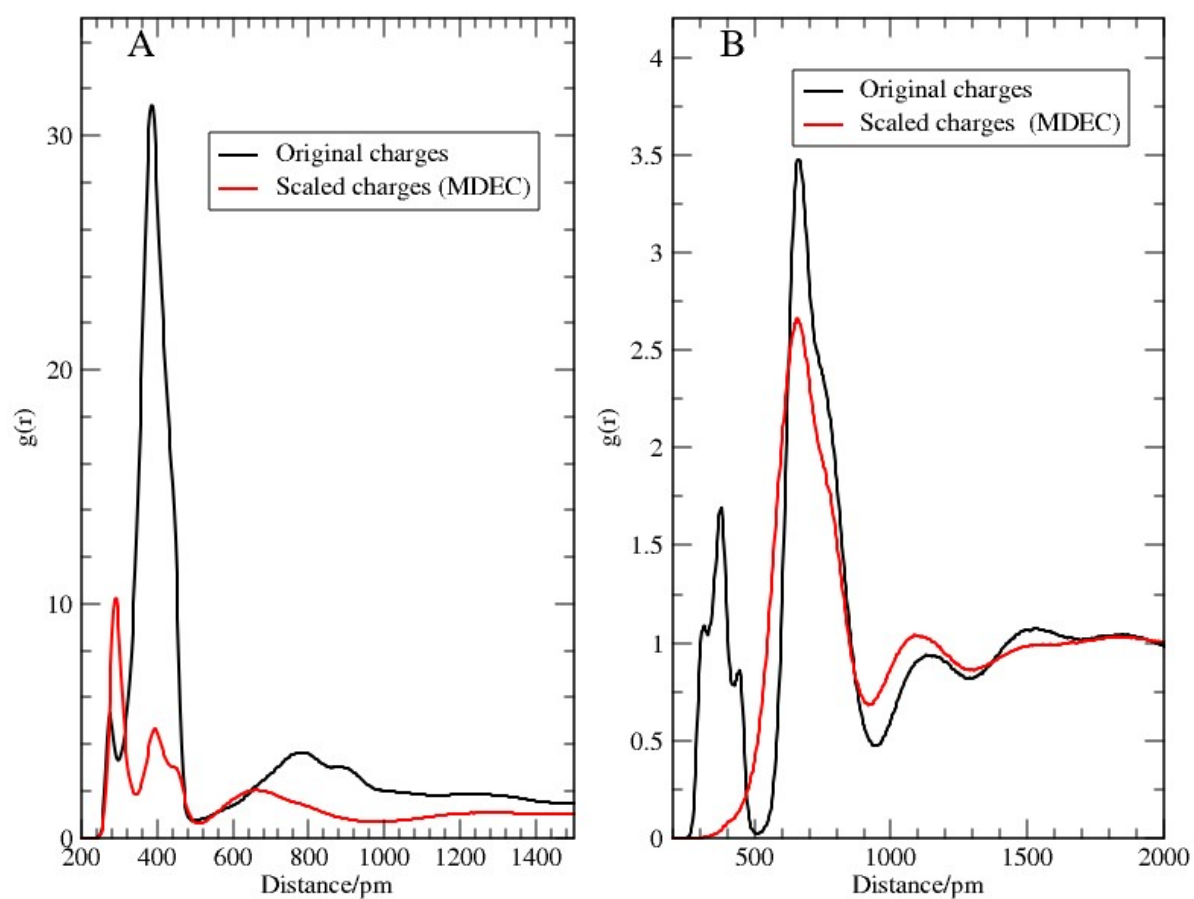


Figure S2: Comparison of the radial distribution functions for FSI-(Center of Mass)/Li<sup>+</sup> for LiFSI solution in CPME (A) and DME (B) using original unscaled charges and scaled charges using the MDEC Method

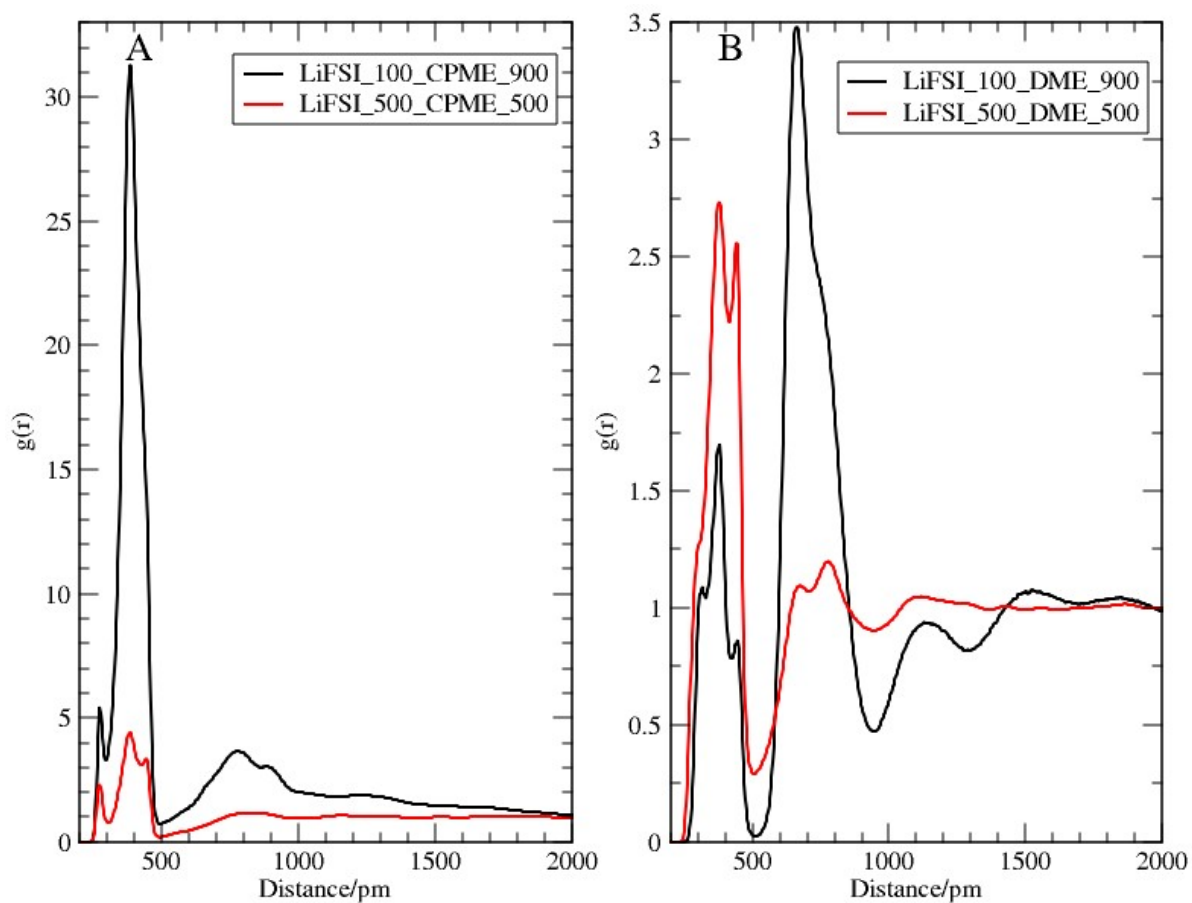


Figure S3: Comparison of the radial distribution functions for FSI-(Center of Mass)/Li<sup>+</sup> for LiFSI solution in CPME (A) and DME (B) using unscaled charges at different concentrations of LiFSI

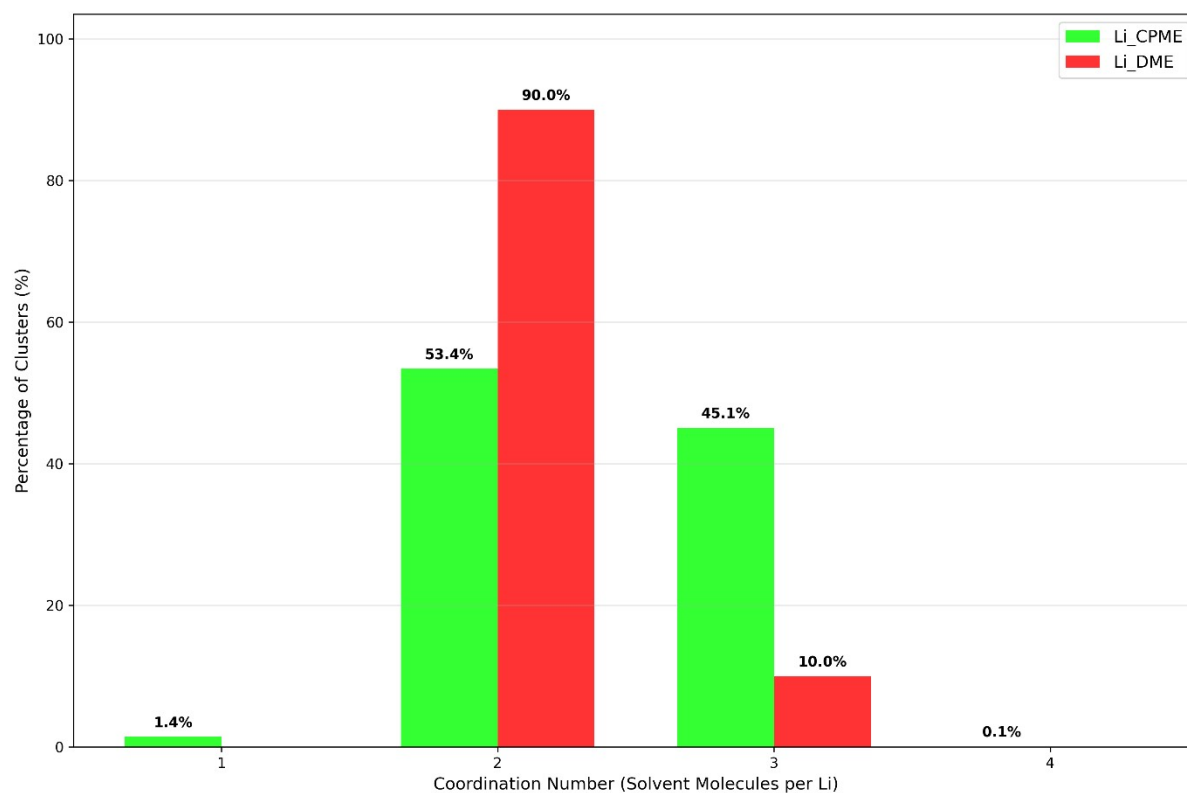


Figure S4:  $\text{Li}^+(\text{SOLVENT})_n$  ( $n=1-4$ ) distribution in 1 M LiFSI solutions in CPME (green) and DME solvent.