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ETHYLENE CARBONATE AND DIMETHYL CARBONATE COMPOSITION DEPENDENCE: A MOLECULAR DYNAMICS STUDY OF Li-IONS IN AN ELECTROLYTE

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Li-ion rechargeable batteries (LIBs) have excellent durability, long cycling life and high specific density. Computational investigation of the effect of temperature, salt concentration and solid electrolyte interface on the Li-ion behaviour has been reported. However, computational studies on the composition dependence of ethylene carbonate (EC) and dimethyl carbonate (DMC) on the Li-ion behaviour are lacking. Here, we study the effect of the entire range of EC and DMC composition in the electrolyte to determine the optimum composition of EC and DMC in Li-ion rechargeable batteries. All systems were represented using the Generalised Amber Force Field (GAFF) and simulated using the LAMMPS code. The following properties were simulated and analysed; density, self-diffusion coefficient, ionic conductivity, cluster formation and ion pair lifetimes. Results showed that all mean square displacements, diffusivities and ionic conductivities increased with increasing DMC mole fraction (χ_{dmc}). Further, irrespective of χ_{dmc}, the highest number of F^- ions and carbonyl oxygen atoms were found, from1.98 to 2.10 Å from Li^+ ions. This indicates the competition among PF_6^- ions and EC and DMC molecules for Li-ions. The system with 0.2 χ_{dmc} showed the highest pair correlation of DMC with Li-ions, while 0.7 χ_{dmc} showed the lowest. The highest pair correlation for EC with Li-ions was observed for 0.4 χ_{dmc}. The incremental increase of χ_{dmc} has increased the diffusivity of Li-ions and, hence the ionic conductivity. It has also shown that Li-EC pair correlation has increased with increasing χ_{dmc} to 0.4, and a further increase in χ_{dmc} has decreased the correlation with Li-ions, indicating that the 0.4 χ_{dmc} as the optimum EC/DMC composition.

Keywords: Dimethyl carbonate, Ethylene carbonate, Li-ion batteries, Molecular dynamics