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Theoretical study of the reductive decomposition of 1, 3- Propane Sultone: SEI forming additive in lithium-ion batteries

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The role of 1,3-Propane Sultone (PS) as an electrolyte additive for lithium ion batteries is explained by investigating the electro reductive decomposition of PS and (PS)Li+$(PC)_n$ (n=0-1) with the aid of density functional theory calculations. In the gas phase, the PS reductive decomposition is thermodynamically unfavorable as supported by the positive Gibbs free energy change and the negative gas phase vertical electron affinity values for the addition of electron to give the radical anion intermediate. However, it is possible that PS can undergo one- as well as two-electron reduction processes in bulk solvent. The origin of this difference is explained by examining the frontier molecular orbital's of PS and its reduction intermediate both in solution and gas phase. A solvated PS is reduced prior to PC to give a stable intermediate which then undergo decomposition to yield a more stable primary radical. The products from the termination reactions of the primary radical (Li_2SO_3, $(CH\text{-}CH_2\text{-}CH_2\text{-}OSO_2Li)_2$, and Li-C carbides) and $(PC\text{-}Li(O_2S)O(CH_2)_3)_2$ from the reduction of (PC)-Li+(PS) would build up an effective SEI film.

Biography

Ermias Girma Leggesse has completed his M.Sc. in Inorganic chemistry from Addis Ababa University and is currently a Ph.D student at National Taiwan University of Science and Technology, Department of Chemical Engineering. He has published one paper in RSC Advances and two papers are under peer review in Journal of power sources.

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