IJARSCT
ISSN (Online) 2581-9429
International Journal of Advanced Research in Science, Communication and Technology (IJARSCT)
International Open-Access, Double-Blind, Peer-Reviewed, Refereed, Multidisciplinary Online Journal
Impact Factor: 6.252
Volume 2, Issue 3, June 2022

Molecular Insights into Battery Electrolyte Stability from a Physicochemical Viewpoint

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Abstract: *Electrolyte stability is a determining factor in performance, safety, and life for rechargeable batteries; this factor will continue to be very important in lithium-ion and emerging high-energy systems. This work adopts a molecular and physicochemical approach for exploring the interplay that exists among solvation structures, ion-pairing, molecular orbital energetics, and interfacial phenomena that will control electrolyte behavior. A mixed-methods approach with experimental investigations complemented by computational simulations was followed. Experimental analyses involved coin cell cycling, electrochemical impedance spectroscopy, and differential scanning calorimetry evaluations of ionic conductivity, capacity retention, coulombic efficiency, and thermal stability across multiple electrolytes. Complementary computational studies involving molecular dynamics and density functional theory simulations have enabled the elucidation of solvation shell configurations, ion-solvent coordination, anion participation, and frontier orbital energy shifts. Preprocessing and multivariate analyses allowed for correlations among molecular descriptors and macroscopic performance metrics. The results are that weakly solvating electrolytes and anion-rich solvation shells bring about substantial enhancements in interphase stability and reductions in solvent decomposition, improving cycle life. For instance, LiTFSI in DOL:DME (3M) exhibited the highest capacity retention at 95% and SEI stability at 91%, while LiDFOB in FEC:DMC (2M) showed superior coulombic efficiency at 99.5%. Results evidence that solvation energy, ion pairing, and electronic structure are critical in determining electrochemical stability and interfacial robustness. These insights provide a framework for rational electrolyte design and optimization of ionic transport, redox stability, and interphase formation. The study here puts in perspective that integration of molecular-level understanding with experimental validation is crucial in guiding next-generation electrolyte development for high-voltage, metal-anode, and long-lifetime applications in battery technologies.*

Keywords: *Electrolyte stability, lithium-ion batteries, molecular design, solvation structure, ion-pairing, HOMO/LUMO, SEI/CEI, weakly solvating electrolytes, thermal stability, interfacial chemistry, high-voltage performance*

DOI: 10.48175/568