

Mechanistic Insight on Solid-Electrolyte Interphase (SEI) Formed by Concentrated Electrolytes Near Lithium Metal

Harender S. Dhatarwal^a, Jer-Lai Kuo^b, and Hemant K. Kashyap^{a,*}

^a*Department of Chemistry, Indian Institute of Technology Delhi, New Delhi 110016, India*

^b*Institute of Atomic and Molecular Sciences, Academia Sinica, Taipei City 10617, Taiwan*

E-mail: hkashyap@chemistry.iitd.ac.in

Concentrated salt solutions are found to be potential electrolytes in lithium metal batteries (LMBs) because of their enhanced electrochemical properties and ultrafast charging–discharging cycles. [1,2] Recently, it has been observed that fluorinated ether-based solvents have extraordinary ability to facilitate the formation of a highly stable ultrathin SEI layer in LMBs.[3] Here, we will discuss the results of our density functional theory based molecular dynamics (DFT-MD) simulations to understand the reductive stability of bis(fluoromethanesulfonyl)imide ([FSI] anion based lithium salt solutions in dimethoxybutane (DMB) and fluorinated dimethoxybutane (FDMB) solvents when they come in contact with lithium metal surface. [4] The mechanism of SEI formation due to dissociation of [Li][FSI]-DMB and [Li][FSI]-FDMB electrolytes, and the composition and distribution of the reduced species over the Li metal anode will also be delineated.[4]

References:

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