Electron and Ion Transport in Li-metal Batteries: Role of the Electrolyte

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Using Lithium as metal anodes is crucial for developing the next-generation of high energy density batteries. However, the high reactivity of Li metal electrodes creates a series of issues that keep them away from practical applications. Electrons are supposed to always travel through external circuits in batteries, however, electron transfer to the electrolyte is the main reason for the formation of a solid-electrolyte interphase (SEI) film, that starts at open circuit conditions. Multicomponent SEI films may have good or not that good passivation properties and a wide range of morphologies depending on the electrolyte. During plating and stripping at the Li metal anode, these events compete with electrolyte decomposition and SEI formation. Thus, at fixed current rate, phenomena such as cation diffusion and desolvation depend strongly on the type of electrolyte and on the stage of formation/consolidation/rupture of the SEI. Here we use first-principles computational tools to analyze the competition between cation electrodeposition and cation solvation-desolvation-decomposition events at Li metal/electrolyte interfaces. We characterize free energy pathways of the cation in various environments and the influence of electrolyte composition and electrochemical stability, and surface structure. We evaluate variables such as the chemistry of the solvent and anion, salt concentration, and presence of additives and their role on facilitating/impeding ion and electron transport at or near the electrode/electrolyte interface.

Bio:

Dr. Perla B. Balbuena is Professor of the Department of Chemical Engineering at Texas A&M University since 2004; she currently holds the Mike O'Connor Chair I. Dr. Balbuena also has joint appointments as Professor of Materials Science and Engineering (since 2006) and Professor of Chemistry at Texas A&M (since 2016). Dr. Balbuena obtained her PhD from the University of Texas at Austin, MSc from the University of Pennsylvania, and BSc from Universidad Tecnologica Nacional, Argentina, all in Chemical Engineering. From 1984 to 1990 she was Associate Professor at Universidad Nacional del Litoral (INTEC) and Associate Researcher of CONICET (Argentina National Research Council). From 1997 to 2004 she was Assistant and then Associate Professor at the University of South Carolina. Her research focuses on first-principles computational materials design, with main areas in interfacial phenomena for batteries, catalysis, and electrocatalysis. She has done pioneering work in computational analysis of lithium ion batteries and fuel cell materials, and has also investigated materials for CO_2 capture, electrocatalysis, and photocatalysis. Dr. Balbuena is author of 326 scientific articles in peer-reviewed journals and has co-edited five books in her areas of specialization. She was elected AAAS Fellow in 2013, and AIChE Fellow in 2020