Theoretical Design of Liquid Electrolytes to Mitigate Dendrite Growth on Lithium Metal Anode

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Lithium metal anode can provide very high energy density when employed in rechargeable batteries such as Li-air and Li-sulfur batteries [1]. However, it has a serious safety issue caused by dendritic growth of Li which leads to the internal short-circuit. While the research of Li dendrite growth has been actively pursued in the previous works [2-7], it is still unclear why dendrite grows and how its morphology can be controlled. In this study, by using simulation tools such as density functional theory calculations, *ab initio* molecular dynamics, and statistical diffusion-limited aggregation modeling, liquid electrolytes have been screened and designed for the mitigation of dendrite growth. Furthermore, theoretically designed liquid electrolytes are tested experimentally by using Li/screened-electrolytes/Li symmetrical cells for measuring short circuit time and *in situ* Li-Li cell for observing dendrite growth directly. Finally, the comparison between theoretical expectations and experimental results will be discussed.

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