

Chitin Fibers as A Nonwoven-Mat Separator for Lithium Metal Batteries: A Computational Study

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The chitin, poly(β -(1,4)-N-acetyl-D-glucosamine), is the second most abundant biogenic macromolecule after cellulose. Herein, we propose the usage of chitin fiber as a nonwoven mat-type separator for lithium metal rechargeable batteries. By theoretical studies with the molecular dynamics simulations and density functional theory calculations, we found that the chitin fiber exhibited the inertness to the aprotic electrolytes and also showed the excellent electrolyte-uptaking capability as compared to the conventional battery separator. In particular, the strong physicochemical affinity to Li-ions with the binding reversibility, which was attributed to the unique coordination with functional groups, was observed. We demonstrated that this chitin-Li-ion interaction could play a critical role in increasing Li-ion movement and alleviating the inhomogeneous distribution of Li-ions at the interface of the electrolyte-absorbed chitin separator and the Li metal anode.