NREL
NATIONAL RENEWABLE ENERGY LABORATORY

Innovation Meets Performance Demands of Advanced Lithium-ion Batteries

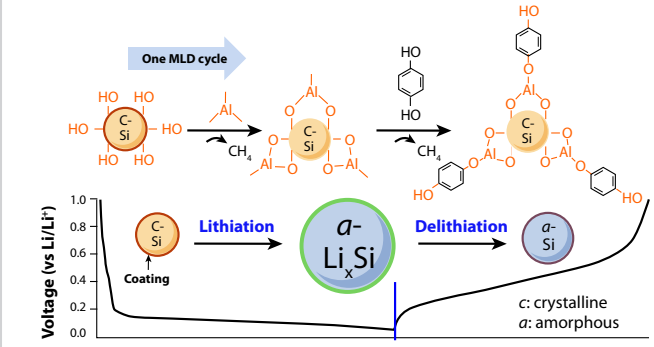
Highlights in Research & Development

Novel surface modification methods are enabling ultrathin coatings to adhere to highly textured battery surfaces.

The growing demand for advanced lithium-ion (Li-ion) batteries, capable of powering high-energy applications and maintaining a lightweight package, has led to NREL's development of methods that introduce surface modification to the electrodes in Li-ion batteries—significantly improving battery cycling stability and lifespan.

NREL researchers and collaborators from the University of Colorado at Boulder have created a breakthrough method for applying ultrathin coatings directly to the electrodes or battery materials with atomic layer deposition (ALD) and molecular layer deposition (MLD). ALD and MLD are state-of-the-art methods that enable ultrathin, conformal coatings to highly textured surfaces, such as complex battery structures.

Advancements in high-capacity and high-energy battery technologies have augmented the need for electrode materials with greater charge capacity and stability. Using ALD and MLD, researchers have demonstrated enhanced cycle life, abuse tolerance, stability, and charge capacity for Li-ion batteries by introducing materials such as metal oxides or hybrid inorganic-organic surface modification.



The schematic of MLD coating for the Si-based materials (top) and the electrochemical lithiation and delithiation of the coated materials (bottom). The MLD coating is based on sequential, self-limiting reactions of trimethylaluminum ($Al(CH_3)_3$) and hydroquinone ($C_6H_4(OH)_2$).

Silicon has emerged as one of the best high-energy anode material options for its low working voltage and high capacity, yet silicon can experience rapid capacity fade from volumetric expansion and solid electrolyte interphase breakdown. A recent NREL study examined how surface modification using MLD may stabilize silicon electrodes in Li-ion batteries. NREL researchers and collaborators demonstrated that a new reaction precursor, the aromatic organic diol hydroquinone combined with trimethylaluminum, led to the flexible surface coating aluminum dioxybenzene, which can accommodate volumetric changes and maintain mechanical integrity of the silicon electrodes.

The combination of mechanical and electrochemical properties achieved with conformal coatings from MLD demonstrates significant advancement in Li-ion technologies. This discovery opens the door for future studies in electro-chemo-mechanics to improve the capacity and stability of Li-ion batteries.

Technical Contact: Chunmei Ban, Chunmei.Ban@nrel.gov

References: Molina Piper, D., Lee, Y., Son, S.B., Evans, T., Lin, F., Nordlund, D., Xiao, X., George, S.M., Lee, S.H., Ban, C. "Cross-Linked Aluminum Dioxybenzene Coating for Stabilization of Silicon Electrodes." *Nano Energy*, 22, pp. 202-210. doi: http://dx.doi.org/10.1016/j.nanoen.2016.02.021.

Key Research Results

Achievement

Advancements in high capacity and high density battery technologies have led to a growing need for battery materials with greater charge capacity and therefore stability. NREL's developments in ALD and MLD allow for thin film coatings to battery composite electrodes, which can improve battery lifespan, high charge capacity, and stability.

Key Result

Silicon, one of the best high-energy anode materials for Li-ion batteries, can experience capacity fade from volumetric expansion. Using ALD and MLD to examine how surface modification could stabilize silicon anode material in Li-ion batteries, researchers discovered a new reaction precursor that leads to a flexible surface coating that accommodates volumetric expansion of silicon electrodes.

Potential Impact

Such developments in ALD and MLD significantly enhance battery performance by mitigating deleterious side reactions and preventing battery materials from degrading over time. The combination of mechanical and electrochemical properties achieved by ALD and MLD may significantly propel advancement in Li-ion battery technologies, improving high-voltage cycling stability and maintaining high capacity.

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15013 Denver West Parkway
Golden, CO 80401
303-275-3000 | www.nrel.gov

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