Thin film high-voltage cathodes for lithium ion batteries

Introduction: Li-ion batteries are the dominant battery technology used in electric vehicles, but wide adoption of batteries in vehicles is hampered by their limited energy density. Therefore research is done on developing a next generation batteries with higher energy densities, which can be achieved by moving towards high-voltage cathodes. However, high operating voltages cause parasitic side reactions and structural changes at the cathode-electrolyte interface, such as the formation of a cathode-electrolyte interphase (CEI) layer on the cathode or the dissolution of transition metal ions into the electrolyte, as shown in **Error! Reference source not found.**. The lack of understanding of the cathode-electrolyte interface is one of the main bottlenecks for the next generation battery technology.

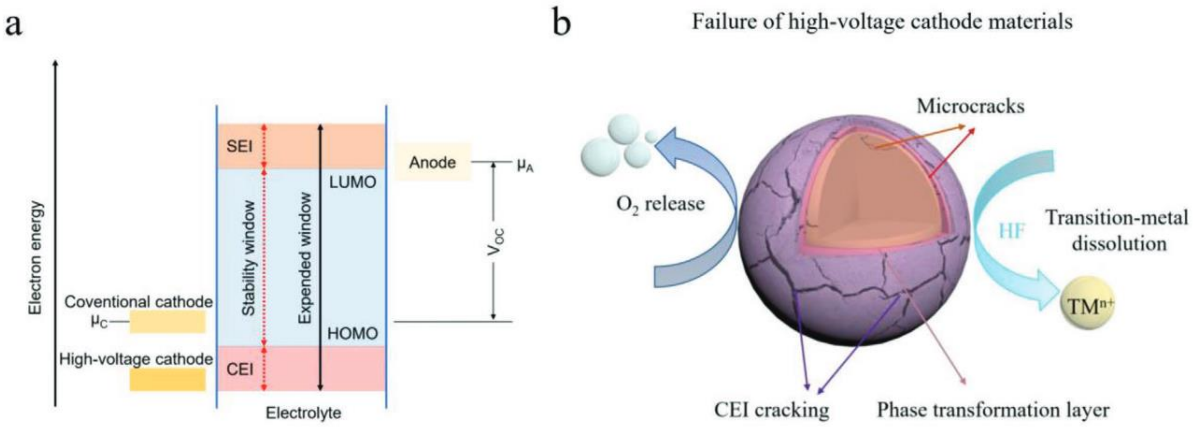

Figure 1. a) The electrochemical potential of high-voltage cathodes lies outside the stability window of liquid electrolytes. b) Degradation mechanisms of high-voltage cathode materials. Figure taken from [1].

Generally Li-ion battery cathodes consist of micron-sized particles mixed with various additives to bind the particles together and improve the conductivity. Within these particle electrodes there is no well-defined interface, so in order to study the cathode-electrolyte interface we use thin film model systems of cathode materials, which are fabricated by atomic layer deposition (ALD). By varying the ALD deposition parameters, the film properties can be tuned. The cathode thin films are used to investigate how the chemical composition and crystallographic properties of high-voltage cathodes affect the interface with (liquid and solid) electrolytes. Secondly, strategies are engineered to create (electro-)chemically and mechanically stable cathode-electrolyte interfaces, such as coating the cathode with an ultra-thin artificial CEI layer.

Project description: Currently research is done on fabricating thin films of high-voltage cathode materials by ALD and on using ALD to deposit artificial CEI layers on particle electrodes to improve their performance. The student will work with us on developing methods to fabricate these materials by ALD, and on characterizing the fabricated materials using techniques such as spectroscopic ellipsometry, X-ray photospectroscopy and X-ray diffraction.

References:

[1] Xiang et al., Advanced materials (2022), 34, 2200912

[2] Donders et al., Journal of the Electrochemical Society (2013), 160, A3066-A3071

[3] Hemmelmann et al., Advanced Materials Interfaces (2021), 8, 2002074

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