Thermodynamics of Artificial Interlayers in Lithium Metal Batteries

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Recent theoretical publications have underlined the importance of interface tailoring in lithium-metal batteries [1]. As most electrolytes are unstable against lithium-metal, artificial interlayers are mandatory [2],[3].
Recently Zhu et al. performed first-principle calculations and identified possible candidates for artificial interlayers in lithium-metal batteries [4]. However, a detailed description of the required properties of these interlayers cannot be found in literature yet, up to our knowledge.
Here we firstly describe the basic thermodynamic concepts of stable and unstable interphases in lithium-metal batteries. Due to the potential difference between the cathode and the lithium-metal anode, a thermodynamic driving force for lithium metal transport exists between the electrodes, which causes several problems with respect to the long-term stability. This potential gradient initiates thermodynamically driven reactions at the interphase between an electrolyte and the lithium metal anode. These decomposition reactions are kinetically hindered, if the electrolyte or the reaction products at the interface have a negligible electronic conductivity.
Possible candidates for artificial interlayers need to have a negligible electronic conductivity to passivate the interface. Another way to protect the interface are sacrificial layers, which react with lithium metal by forming products with a high ionic conductivity and a negligible electronic conductivity (e.g. LiPON).

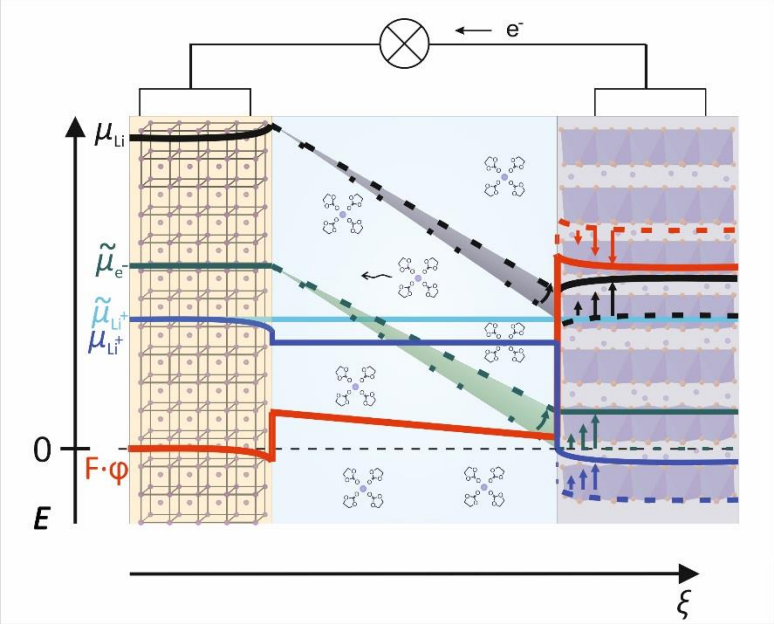

Fig. 1: Qualitative representation of basic thermodynamic quantities in a battery with a lithium-metal anode, a lithium cobalt oxide cathode and a liquid electrolyte.

References:

[1] Y. Zhu, X. He, Y. Mo, ACS Appl. Mater. Interfaces 7 (2015) 23685-23693
[2] S. Wenzel, T. Leichtweiss, D. Krüger, J. Sann, J. Janek, Solid State Ionics 278 (2015) 98-105.
[3] S. Wenzel, D.A. Weber, T. Leichtweiss, M.R. Busche, J. Sann, J. Janek, Solid State Ionics 286 (2016) 24-33.
[4] Y. Zhu, X. He, Y. Mo, Adv. Sci. (2017) 1600517