Materials and reaction mechanisms in beyond intercalation batteries

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Abstract

My research interests embrace the development of new materials for beyond intercalation batteries and the understanding of the physicochemical processes in the working environment. Particular chemistries involve metal-O_2, metal-S, alloying, and capacitive materials. Here, I address recent advances in three directions. (I) Soft mixed electron/ion conductors. (II) The highly reactive singlet oxygen in battery chemistries. It is intimately tied to oxygen redox chemistries where O_2 is evolved at some point. I discuss the set of methods we developed for its identification. With respect to metal-O_2 cells we could reveal that it accounts for the majority of the parasitic reactions. We further report on the formation mechanism, materials stability, a new class of high-voltage stable quenchers, and ways to suppress its formation. Moreover, $^1O_2$ forms upon oxidizing Li_2CO_3 above 3.8 V vs Li/Li^+ which makes it relevant for most cathodes. (III) Phase evolution in metal-O_2 and metal-S cells. I present operando small and wide angle X-ray scattering as a powerful real-time in situ metrology tool with structural information at the atomic to micron level. For data analysis, a recently developed method is combined with a nucleation and growth model in a realistic 3D carbon pore model. Together, this allows for new insights into reaction mechanisms and to derive design criteria for materials.

Biography

Stefan Freunberger obtained his PhD in Chemistry from ETH Zürich and was post doc at the University of St Andrews, working on many aspects of Li-O_2 chemistry. He is now PI at Graz University of Technology, Austria, with research interests embracing energy-storage materials, including alkaline-ion and metal-O_2 batteries, electrolytes, and in situ techniques.