Abstract #1233, Honolulu PRiME 2012, © 2012 The Electrochemical Society

# Tailored Redox Shuttle Additives for Overcharge Protection of Lithium-Ion Batteries

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Chemical shuttles are essentially organic compounds which can be reversibly oxidized / reduced at an intrinsic redox potential. Among their many applications, overcharge protection for lithium-ion batteries is the most significant one (1-6).

Generally, the redox shuttle molecule can be reversibly oxidized and reduced, as shown in Figure 1, at a defined potential slightly higher than the end-of-charge potential of the positive electrodes. When the positive electrode is overcharged, the redox shuttle molecule (RS) would be oxidized to its (radical) cation form (RS·+), which, via fast diffusion across the electrolyte, would be reduced to its original state on the surface of the negative electrode. The reduced form would then diffuse back to the positive electrode to get oxidized again. The "oxidation-diffusion-reduction-diffusion" cycle could be repeated continuously due to the reversible nature of the redox shuttle to shunt the overcharge current and protect the positive electrode from damaging. Figure 2 illustrates this mechanism of the overcharge protection of $LiFePO_4$ cell using Argonne's new discovered redox shuttle.

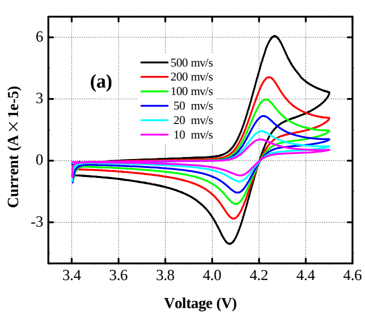


**Figure 1.** Typical cyclic voltammetry profile of a redox shuttle additive.

The electrolyte research group at Argonne National Laboratory has designed, synthesized and characterized a couple of categories of new chemical shuttles and investigated their performance as overcharging protection additives. One category belongs to aromatic compounds bearing a benzene ring in the structure. By introduction of various functional groups onto the benzene ring generated shuttle molecules with tailored redox potentials.

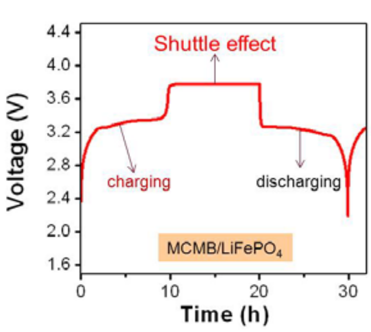


**Figure 2.** Representative voltage profile of a MCMB/$LiFePO_4$ cell using Argonne's new redox shuttle.

In this talk, one specific shuttle molecule for $LiFePO_4$ will be thoroughly presented in terms of molecular design (Figure 3), solubility; overcharge stability et al. High voltage redox shuttles will also be discussed for the application of other lithium ion battery chemistries including 4.0V $LiMO_2$ cell and 5.0V high voltage cathode cell.

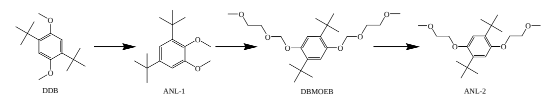


**Figure 3.** Molecular design of redox shuttle additives for $LiFePO_4$ cells.

## References

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