

Redox Active Molecular Engineer for Energy Storage

Lu Zhang, John Vaughey, Anthony K. Burrell

Argonne National Lab

Abstract:

Organic redox active or reversible molecules are usually built upon conjugated systems, which could help stabilize the radicals and ions generated during redox process, therefore most of them could go back and forth from difference redox states to their neutral states upon external electrochemical control or stimulus. This unique reversible behavior makes them of extreme interest to electrochemical energy storage and leads to many possible applications in various technologies.

Molecular engineer of organic redox active molecules could lead to tunable physical and electrochemical properties, including solubility in organic solvents, molecular mobility, redox potential, and electrochemical reversibility, which are key factors to energy storage applications. Specifically, one family of dimethoxybenzene based organic molecules will be discussed in this talk. Dimethoxybenzene based molecules have drawn increasing attentions due to their excellent electrochemical activities, especially as redox shuttle additives and possible non-aqueous flow battery catholytes, which both require redox active molecules to be the key functional components. Due to the organic synthesis feasibility, structural improvements could be conducted to intentionally tune the physical or electrochemical properties of dimethoxybenzene. For instance, ANL-2 was developed with improved solubility in carbonate based electrolytes and excellent overcharge performance as redox shuttle additive. The success of ANL-2 was based on the previous attempts using various design strategies to improve the solubility of DDB, including asymmetric ANL-1, and DBMOEB (1,4-di-tert-butyl-2,5-bis(2-methoxyethoxy)methoxybenzene). Other examples are ANL-3 and ANL-4 molecules, with focus on increasing the redox potentials. ANL-3 is able to provide 4.8 V vs Li/Li⁺ overcharge protection, highest ever reported in the literature. ANL-4, on the other hand, exhibited 4.5 V vs Li/Li⁺ redox potential and good electrochemical reversibility.

