

# SPECIAL SEMINAR

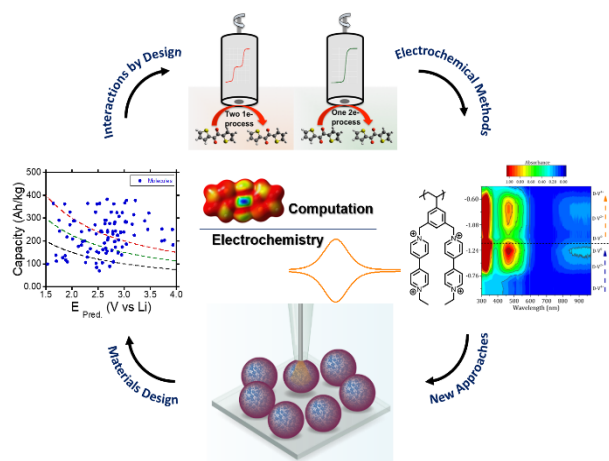
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*“Enhancing charge transfer through molecular design:  
From small molecules to polymers”*

An important challenge for enabling the wide-spread utilization of renewable energy sources, such as solar and wind, is the development of high efficiency, low cost, high energy density, safe, and environmentally benign electrochemical energy storage (EES) technologies. Among the different types of EES technologies, metal ion batteries and redox flow cell batteries are attractive alternatives for grid energy storage. Organic compounds represent attractive alternatives as electrode materials for batteries due to their well-known redox chemistry as well as the variety of redox-active functional groups that can be studied. In my talk, I will discuss how I have combined computational and electrochemical methods for the design and characterization of new organic-based materials for EES applications. Computational methods were used to predict the formal potentials of new materials to enable the identification and down-selection of the most promising candidates. With experimental methods we found that a metal cations shifted the redox to more positive potentials, thus enhancing in that way the energy density of the materials. My current research focuses on the use of redox active polymers (RAPs) for non-aqueous redox flow batteries. Presently, measuring the electron transfer kinetics of large mediators with hundreds of redox active centers is not well understood. In this seminar, I will discuss the different electrochemical techniques that we used for the characterization of small redox molecules and RAPs. From these studies, we learned that charge hopping and electron self-exchange between neighboring pendants and redox kinetics impact the charge/discharge performance of organic materials.



**Fig. 1.** Schematic representation of my research career where I combined computational methods and electroanalytical techniques for the characterization of new materials.

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Chemistry