The Understanding of Molecular Recognitions Drives the Discovery of Novel Materials

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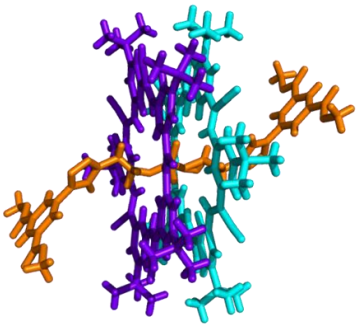
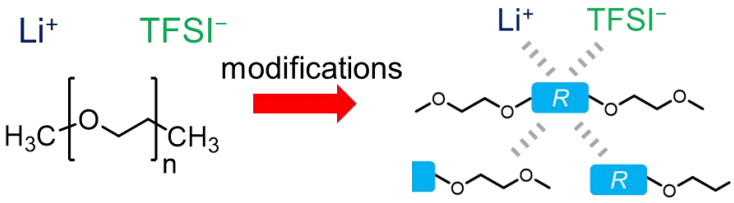
Non-covalent interactions are widely used in developing materials with unique properties such as high-fidelity recognition, self-healing, and stimuli responsiveness. In this talk, I will share two stories of understanding and utilizing non-covalent interactions in the context of developing novel materials. The first story is about taking advantage of the selective and cooperative recognition of a wide variety of anions by shape-persistent macrocycles in the supramolecular synthesis hierarchical self-assemblies. These self-assembled structures demonstrate interesting optical and acid-base response properties. The second story focuses on developing a quantitative and easy-to-execute framework that allows us to understand and predict the substituent effects in oligoethylene oxide (OEG) based lithium electrolytes. In this work, molecular level non-covalent interaction energies are successfully used as substituent parameters to fit the experimental data and to predict the macroscopic properties (conductivity, viscosity, and glass transition temperature) of OEGs modified by a variety of substituents.



Using anion recognition in supramolecular syntheses



Understanding the impact of non-covalent interactions on lithium conduction