Designing Hysteresis Free High-Valent Redox for Electrochemical Applications

Advances in electrochemical devices such as batteries, fuel cells, and water-splitting membranes are driving the global transition towards clean and renewable energy. Foundational to (electro)chemical and catalytic transformations in these devices is a stable and reversible high-valent redox couple. In particular, the phenomenon of high-valent oxygen redox (anionic redox) in lithium- and sodium-ion positive electrodes has the potential to significantly increase energy density by providing additional high voltage capacity beyond that of most transition metal redox couples. However, the additional capacity from anionic redox comes at the expense of reduced reversibility in the form of voltage hysteresis and voltage fade. As a result, reversible high-valent redox couples have long been thought to be impossible. In this seminar, I will 1) discuss the mechanism and the framework for understanding the source of poor electrochemical reversibility in high-valent redox; 2) demonstrate a mechanism to avoid structural disorder and voltage hysteresis; 3) suggest a set of practical design rules to engineer materials with reversible high-valent redox. My work lays a foundation to effectively harness the untapped benefits of high-valent redox materials for vast application areas including electrochemical energy and data storage, catalysis and sensing.

Iwnetim (Tim) Abate is a DARE Doctoral Fellow in Materials Science & Engineering at Stanford University. He is co-advised by Prof. William Chueh and Prof. Thomas Devereaux. His research aims at improving the energy capacity of batteries to meet the ever-growing global demand for energy storage. His work combines X-ray and electrochemical characterization with quantum mechanical simulations to design next generation lithium- and sodium-ion batteries. Prior to joining Stanford, he did a research stint at IBM Alamden and Los Alamos National Laboratory.

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