Materials Alchemy: Unlocking Energy Storage Potentials through Structural Understanding

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The repercussions of global climate change are intricately linked with the extraction of fossil fuels, necessitating a shift towards energy harvesting from renewable sources. The intermittent nature of these renewables underscores the need for efficient storage systems to cater to off-hours demand. In contemporary energy storage systems, there has been a significant and transformative transition from conventional stationary storage to transportation-oriented solutions. To keep pace with these evolving demands, the design of new materials requires timely intervention. This involves a radical shift from lab-based synthesis to the adoption of cutting-edge techniques for characterization, subsequently extending to industrial implementations.

The high energy density and environmentally friendly nature of hydrogen make it a viable alternative to fossil fuels. In this context, the conversion of solar power to H_2 and synfuels, utilizing H_2O and CO_2, appears to be a sound option. In my talk, I will discuss the role of Mn-based perovskite oxides in reducing the thermal conversion temperature of H_2O to H_2.[1] Reactions of this nature involved constructing a lab-based reactor coupled with a water evaporator and gas detectors. I will elaborate on how we navigated towards hitherto new materials by correlating these reaction temperatures and rates with the local structural parameters of the perovskites.[2]
Given their significant power density, extended cycle lives, and rapid charge-discharge rates, lithium-ion batteries (LIBs) have been recognized as the most attractive energy storage technologies. However, they may not be the most suitable candidate to replace fossil fuels in achieving the net-zero carbon goal of this century due to the non-abundancy of lithium (18 ppm in the Earth's bedrock and 0.2 g/m³ in saltwater).[3] Research into alternative battery chemistries, such as magnesium-ion batteries (MIBs), which benefit from abundance and compete favorably in energy density profiles with LIBs, has seen promising advances. In my talk, I will discuss my recent work on Mg-ion cathodes, spanning transition metal sulfides, oxides, polyanion, and elemental sulfur systems. A suite of short- and long-range techniques as employed to track the ion intercalation-deintercalation mechanism (including operando techniques) in these materials, will be discussed.[4, 5] Furthermore, I will discuss about the unusual anion redox and simultaneous cation-anion redoxes observed in advanced Mg and Li ion batteries.[6] To conclude, I will briefly outline a portion of my future plans in the context of research and teaching activities.

(1) Rao, C. N. R. et. al., *PNAS* 114.51 (2017): 13385-13393.
(2) Dey, S et al., *Chem. Eur. J.* 21.19 (2015): 7077-7081.
(3) Bieker, G. et al., *Communications Materials* 2.1 (2021): 37.
(4) Dey, S. et al., *JACS*, 142.46 (2020): 19588-19601.
(5) Blázquez, J. A. et al., *Energy & Environ. Sci.*, 16.5 (2023): 1964-1981.
(6) Dey, S. et al., *Chem. Mater.* 33.11 (2021): 3989-4005.