

MATERIALS AND BIOMATERIALS SCIENCE AND ENGINEERING**Negative Charge Transfer: Ground State Precursor
towards High Energy Batteries**

ABSTRACT: Modern energy applications, especially electric vehicles, demand high energy batteries. However, despite decades of intensive efforts, the highest energy density and commercially viable batteries are still based on LiCoO_2 , the very first generation of cathode materials. The technical bottleneck is the stability of oxide-based cathodes at high operating voltages. The fundamental puzzle is that we actually never understood the redox mechanism of LiCoO_2 . Conventional wisdom generally defines redox to be centered on cations at low voltages, and on anions, i.e. oxygen, at high voltages by forming oxidized chemical states like O_2 or peroxo-species. In this talk, through in-situ and ex-situ spectroscopy coupled with theoretical calculations, we show that high-energy layered cathodes, represented by LiCoO_2 and LiNiO_2 , operate through enhancement of negative charge transfer (NCT) ground states upon charging throughout the whole voltage range - i.e., NCT evolution itself is the intrinsic redox mechanism regardless of voltage ranges. NCT inherently engages high covalency and oxygen holes, leading to optimized performance without conventional redox centers in LiCoO_2 . The level of NCT, i.e., number of ligand holes, naturally explains many seemingly controversial results. The redefinition of redox mechanism reveals the pathway toward viable high energy battery electrodes.

BIOGRAPHY

Thomas Devereaux is a professor of Materials Science & Engineering and Photon Science at Stanford University and SLAC National Accelerator Laboratory. He received his Ph.D. in Physics from the University of Oregon, and was a postdoctoral fellow at the Max Planck Institut, Stuttgart and University of California, Davis. Professor Devereaux's research interests are focused on understanding equilibrium and ultrafast non-equilibrium electron dynamics via a combination of analytical theory and numerical simulations to provide insight into materials of relevance to energy science. The specific focus of the group is the development of numerical methods and theories of photon-based spectroscopies of strongly correlated quantum materials and novel materials for energy storage.

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Refreshments: 1:45pm, Seminar: 2-3pm