MS18-02 | Order-Disorder Transitions in Battery Electrodes Studied by Operando X-ray Scattering

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Development of novel electrode materials for intercalation type batteries have in the past focused on highly crystalline materials with the capability to retain long-range order during cycling. However, recent years have seen an increased interest for disordered materials, e.g. with the discovery of multiple high capacity electrodes based on disordered rock-salt structures or even completely amorphous materials exhibiting higher capacities than their crystalline counterparts.[1] Furthermore, it was recently showed by Ceder et al that long-range order is not a prerequisite for maintaining percolating intercalation pathways.[2] Still very little is known about the structural mechanisms behind order-disorder transitions induced by ion-intercalation or about ion-storage mechanisms in disordered materials.

Using a combination of operando synchrotron X-ray diffraction and total scattering (with pair distribution function analysis), we have studied a series of disordered and amorphous electrode materials such as nano-rutile TiO_2, V_2O_5, and various MnOx-polymorphs [4]. This allows us to map out the structural evolution during battery charge and discharge at the atomic- and nano-scale, and begin to understand the ion-storage mechanisms in such materials. In this presentation, we will focus on results which demonstrate the different types of order-disorder phenomena (e.g. topotactic, reconstructive, domain size reduction) and ion-storage mechanisms (e.g. solid solution, two-phase transition) we have encountered.

[1] J. Lee et al., Nature 2018, 556, 185-190.; E. Uchaker et al., J. Mater. Chem. A 2014, 2, 18208-18214.
[2] J. Lee et al., Science 2014, 343, 519-522.
[3] C. K. Christensen et al., Chem. Mater. (2019) DOI: 10.1021/acs.chemmater.8b04558.