Das Research Group

We employ various theoretical methods to understand the origin of the macroscopic properties of materials at the atomic level. We aim to explore the complex interplay between the crystal structure, materials chemistry and various microscopic degrees of freedom that lead to the emergence of various quantum phenomena, since this is the first fundamental step in the designing of new materials with new and/or enhanced functionalities. Our long-term goal is to design new materials where the desired quantum phenomena can be realized. The nature of our work is highly collaborative, with a tight feedback loop between first-principles predictions, synthesis of candidate materials, and advanced characterization of emergent properties. We endeavor to address a wide variety of emergent properties of quantum materials with applications ranging from advanced electronics to clean energy production.

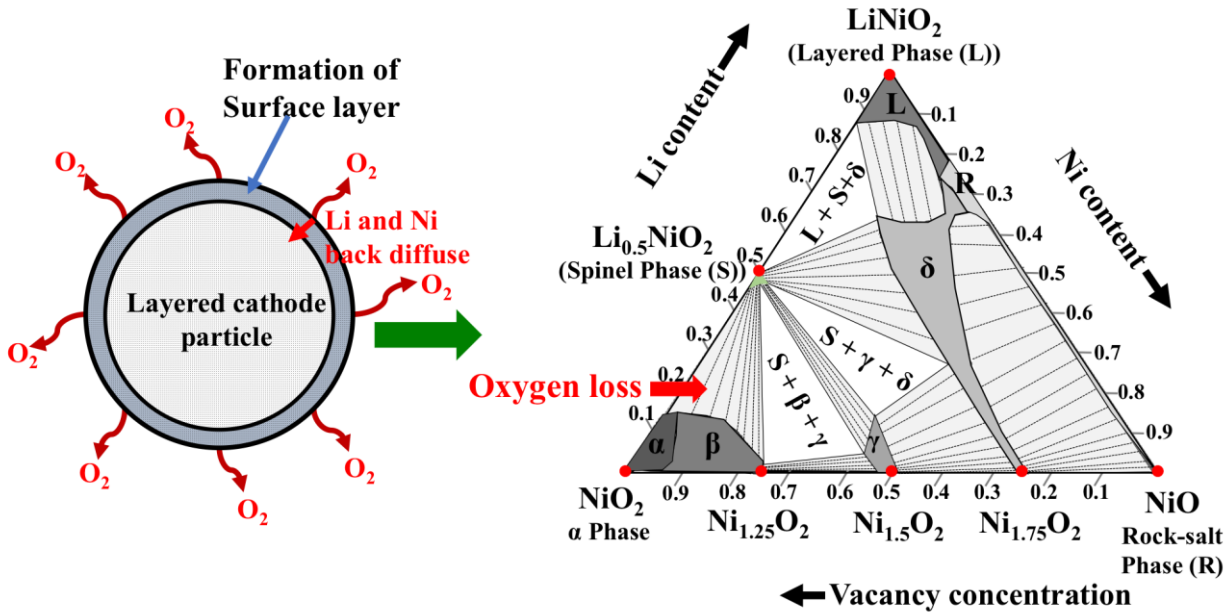

Figure 1: Based on a material specific lattice Hamiltonian and Grand Canonical Monte Carlo simulations, we have predicted several new structural phases of $Li_xNi_xO_2$ system within a fixed fcc anion lattice which form during battery charge-discharge process [*Chem. Mater.* ***29****, 7840 (2017)*] and these phases have a significant bearing upon the performance of Li-ion cathode materials.

To achieve our research goals, we use a combination of theoretical tools like, Density Functional Theory (DFT) based electronic structure methods, group theoretic techniques, microscopic models and various Monte Carlo simulation techniques.

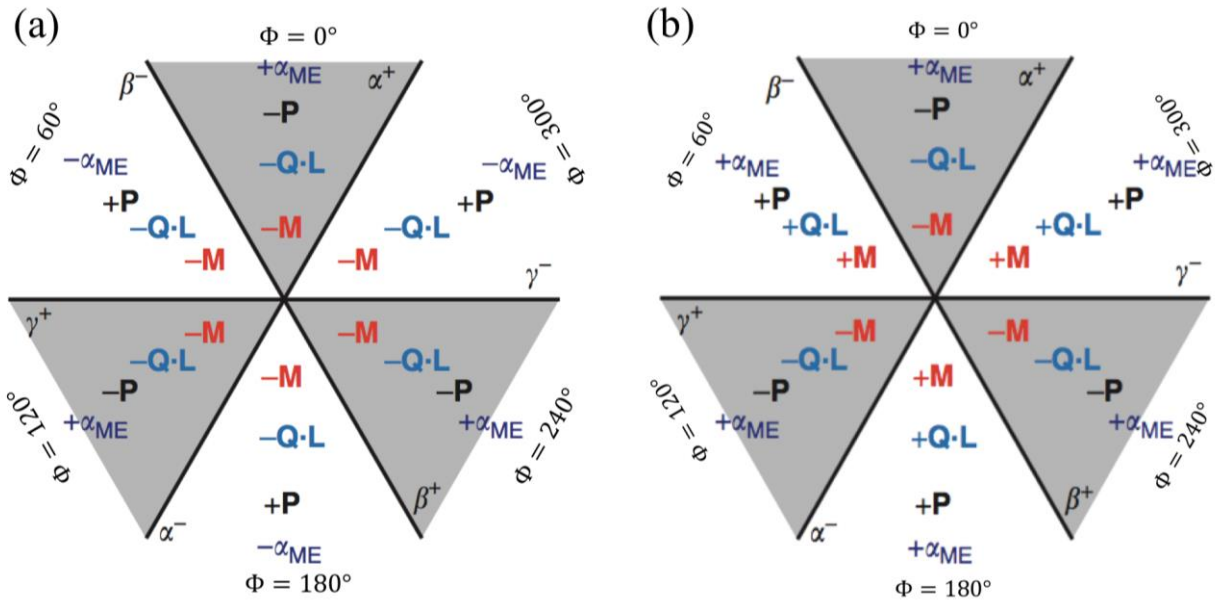

Figure 2: We showed that within $YMnO_3$ hexagonal structural motif, a non-polar lattice distortion that trimerizes the unit cell size leads to the formation of a bulk linear magnetoelectric (ME) vortex domain structure (a) or a bulk ME coupling such that if the direction of the polarization was reversed so did the direction of magnetization (b) [*Nature Communications* ***5****, 2998 (2014), Nature Materials* ***13****, 163-167 (2014)*].