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Structure, morphology and stability of layered $\text{Li}(\text{Ni}_{1/3}\text{Mn}_{1/3}\text{Co}_{1/3})\text{O}_2$ surfaces JUAN GARCIA, Materials Science Division, Argonne National Laboratory, JAVIER BARENO, Chemical Sciences and Engineering Division, Argonne National Laboratory, GUOYING CHEN, Energy Storage Group, Lawrence Berkeley National Laboratory, JASON CROY, Chemical Sciences and Engineering Division, Argonne National Laboratory, HAKIM IDDIR, Materials Science Division, Argonne National Laboratory — Energy storage devices with high energy densities are needed in order to meet the increasing demands of portable electronics and electric vehicles. Layered $\text{Li}(\text{Ni}_{1-x-y}\text{Mn}_x\text{Co}_y)\text{O}_2$ (NMC) oxides are promising cathode materials that are capable of meeting many of these demands. However, in order to take advantage of these high intrinsic energies, charging voltages of $>4.2\text{V}$ (vs. graphite) are necessary. At such high voltages, surface degradation phenomena take place at untenable rates, thereby reducing the lifetime of cells. In order to take advantage of NMC-based Li-ion cells, the mechanisms of these surface degradation processes must be fully understood. This presentation will explore recent Density Functional Theory (DFT) efforts at Argonne National Laboratory aimed at predicting the stability of several low-index surfaces of $\text{Li}(\text{Ni}_{1/3}\text{Mn}_{1/3}\text{Co}_{1/3})\text{O}_2$ (NMC-111) as a function of Li and O chemical potentials. Comparison will be made of predicted particle shapes with those of single-crystal NMCs synthesized under different conditions. The most stable surfaces for stoichiometric NMC-111 will be discussed in terms of polar and non-polar surfaces as well as metal-oxygen bond breaking. The reactivity of these surfaces toward electrolyte oxidation will also be presented.

Hakim Iddir
Materials Science Division, Argonne National Laboratory

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