Study of sodium containing layered oxides for battery applications: Defect control to enhance ionic conductivity

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Abstract: The goal of this project is to develop sodium-containing novel layered honeycomb oxides for solid state battery cathodes. A combined experimental and theoretical effort was undertaken by our team to discover alternatives to replace critical elements like lithium (Li) and cobalt (Co) which are currently routinely used in solid state secondary batteries for energy storage. An economically and environmentally viable solution is to use sodium (Na) or other alkalis to replace the critical elements. We explored the family of compounds $A_2M_2TeO_6$ (A = alkali, M = transition metal) in this project. Our preliminary results include successful synthesis of several $Na_2Ni_2TeO_6$-derived compounds with varying Na content (i.e. cationic vacancies) and substitutions (ex. Zn replacing Na). The motivation for the chemical tuning is the close connection between defect structure and ionic conductivity in the proposed compounds. We are working on the quantification of the optimal Na-content for highest ionic conductivity in the proposed compounds. Density functional theory (DFT) calculations were carried out to investigate the most favorable chemical coordination around Na ions which supports optimal ionic conduction. Our preliminary DFT result shows good agreement between calculated and measured lattice constants, predicting the bulk modulus to be 98 GPa and 97 GPa for $Na_2Ni_2TeO_6$ and $Na_3Ni_2TeO_6$, respectively. DFT calculations for three different sodium sites (i.e., Na1, Na2, and Na3) in $Na_2Ni_2TeO_6$ were conducted. Our results indicate that Na atoms in the Na1 site are energetically more favorable than the ones either in Na2 or in Na3 sites. This finding agrees well with the measured XRD data. Structural and magnetic properties were also investigated.