

An *ab initio* study on multi-principle-element layered oxides as cathode materials in Li ion batteries

Che-an Lin, Ralph N. Nasara, and Shih-kang Lin*

Department of Materials Science and Engineering, National Cheng Kung University,
Tainan, Taiwan

*Corresponding author: linsk@mail.ncku.edu.tw (S.-k. L.)

NMC is one of the most widely used layered cathode in lithium-ion batteries due to its high theoretical capacity and voltage. However, the stability of NMC at a high state of charge has always been a significant concern for people. Its stability limits its usable capacity which is relatively low compared to its theoretical capacity. To increase the efficiency of NMC, considerable approaches have been carried out, such as changing the proportion of transition metals, doping, and making it into composite material. Although many doping elements can improve the properties of NMC, the amount of doping is often limited due to second phase formation. Utilizing the concept of multi-component material, the formation energy changes due to the number and proportion of elements, we designed a layered cathode with five elements in the transition metal layer, which includes Ni, Mn, Co, and two extra elements, to not only get benefits from the addition of extra elements but also maintain single phase at the same time. Ti, V, Cr, and Al were chosen to be investigated as extra elements according to their valence states and ionic radii. We systematically built the model according to the atom arrangement and radial distribution function, and decided the most reasonable model by calculating their formation energy with *ab initio* calculation. After building a reasonable model for the multi-component layered cathode, we simulated the reaction during delithiation to provide an examination of its stability at different state of charge.