Analysis of voltage profile of $NaMnO_2$ cathode using DFT+U/linear response computational method

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$NaMnO_2$ is a cathode material, featured by a high operating voltage, reasonable capacity and stability to electrochemical cycling [1]. Material structure of $NaMnO_2$ allows two types of polymorphs (α and β), which are known to coexist in synthesized materials. While such intergrowth of α and β polymorphs has been studied in the past [2], a detailed computational analysis of voltage dependence from Na concentration in such compounds is still missing.

In this work we employ DFT+*U*/linear response calculations [3] to study voltage profiles for pure α and β polymorphs and also for intermixed α and β structure (Figure 1). Our study shows that the voltage profile of β and intermixed models can be calculated in a very reasonable agreement with experiment. We also analyze formation of structural defects at low concentration of Na and discuss their role in voltage decay and capacity fade.

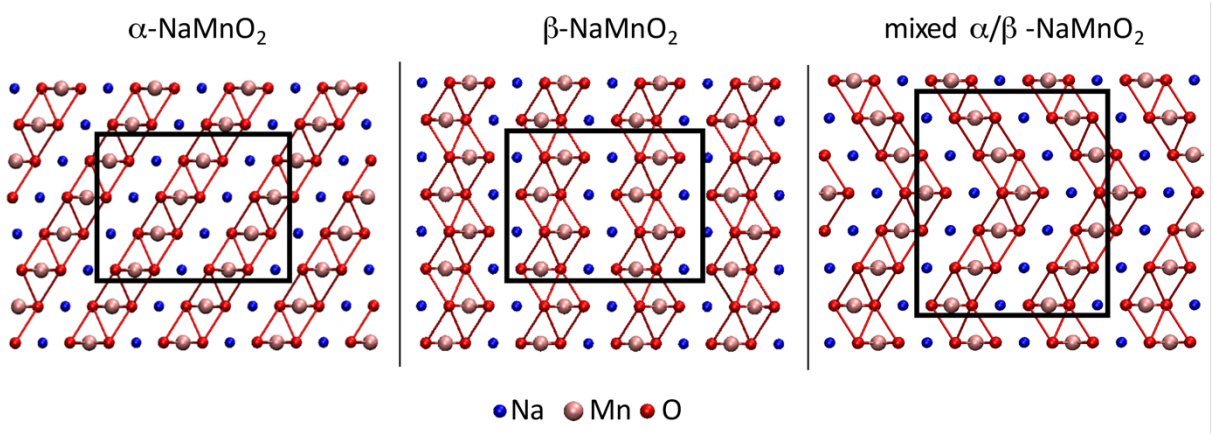

Figure 1 The structures of α, β and intermixed α/β $NaMnO_2$. Computational cells, used in calculations are indicated by the black solid line rectangles.

References:

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