Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Polaronic and ionic conduction in $NaMnO_2$: influence of native point defects ZHEN ZHU, HARTWIN PEELAERS, CHRIS G. VAN DE WALLE, Materials Department, University of California, Santa Barbara — Layered $NaMnO_2$ has promising applications as a cathode material for sodium ion batteries. We will discuss strategies to improve the electrical performance of $NaMnO_2$, including how to optimize the conditions of synthesis and how impurity doping affects the performance. Using hybrid density functional theory, we explored the structural, electronic, and defect properties of bulk $NaMnO_2$. It is antiferromagnetic in the ground state with a band gap of 3.75 eV. Small hole and electron polarons can form in the bulk either through self-trapping or adjacent to point defects. We find that both Na and Mn vacancies are shallow acceptors with the induced holes trapped as small polarons, while O vacancies are deep defect centers. Cation antisites, especially Mn_{Na}, are found to have low formation energies. As a result, we expect that Mn_{Na} exists in as-grown $NaMnO_2$ in moderate concentrations, rather than forming only at a later stage of the charging process, at which point it causes undesirable structural phase transitions. Both electronic conduction, via polaron hopping, and ionic conduction, through V_{Na} migration, are significantly affected by the presence of point defects. This work was supported by DOE.

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Date submitted: 08 Nov 2016 Electronic form version 1.4