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Computational studies of Na/MgMn₂O₄ Spinels.

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Spinel lithium manganese (II) oxide (IV) (LiMn₂O₄) has been intensively studied as a positive electrode for rechargeable Li-ion batteries due to its abundance in the earth crust, low toxicity, and high theoretical capacity of 148 mAh/g. However this material has been reported to suffer from severe capacity fading, particularly at high temperatures during the charge/discharge process. This drawback makes the material incompetent for commercial application, though many attempts were made to improve its capacity sustainability. Recently, preliminary studies have shown that NaMn₂O₄ and MgMn₂O₄ have great potential for use in Na-ion and Mg-ion batteries. However, little has been reported on the physical and chemical properties of these compounds.
In this work, we perform first principles calculations to investigate the structural, thermodynamic, electronic and mechanical properties of NaMn₂O₄ and MgMn₂O₄, particularly the lattice constants, heats of formations, band structure, density of states, elastic constants and phonon dispersion curves. Furthermore, the operating voltages are also calculated. Calculations have been performed within DFT+U method as implemented in the Vienna Ab initio Simulation Package code. The calculated lattice constants are in good agreement with the experimental data to within 3 %. The electronic DOS and band structure calculations suggest that NaMn₂O₄ and MgMn₂O₄ are conductors due to the absence of energy band gap around the fermi level.

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