Through synthesis and computation, transition-metal substituted layered electrode materials for Na-ion batteries are explored: when partially substituted with titanium, improvements on structural stability, charge transfer ability, and electrochemical properties with respect to high-voltage stability and total reversible capacity are observed.

Significance and Impact

Na-ion batteries are of great interest for the next generation of energy storage, as their materials are highly abundant and efficient. This work provides insights towards the essential structural chemistry of high-capacity, low-cost layered electrodes for NIBs.

Research Details

Layered compounds with different stacking modes, O3-Na$_{2/3}$Mg$_{1/3}$Ti$_{1/6}$Mn$_{1/2}$O$_2$ and P2-Na$_{2/3}$Mg$_{1/3}$Mn$_{2/3}$O$_2$, were studied via DFT calculations and electrochemical measurement.

- The decreased Mg and Mn ordering distribution is observed in TMO$_2$ layers.
- Ti substitution facilitates charge-transfer reaction of oxygen redox.
- The highly stable high-voltage plateau is exhibited at $\sim$4.1 V.