Ni and Fe substituted Mn-based P2-type layered oxide cathode for high energy density sodium-ion battery

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Herein, a new P2-type layered oxide is proposed as an outstanding intercalation cathode material for high energy density sodium-ion batteries (SIBs). Based on the stoichiometry of sodium and transition metals, the P2-type $Na_{0.55}[N_{0.1}Fe_{0.1}Mn_{0.8}]O_2$ cathode is synthesized without impurities phase by partially substituting N and Fe into the Mn sites. The partial substitution results in a smoothing of the electrochemical charge/discharge profiles and thus greatly improves the battery performance. The P2-type $Na_{0.55}[N_{0.1}Fe_{0.1}Mn_{0.8}]O_2$ cathode delivers an extremely high discharge capacity of 221.5 mAh g^{-1} with a high average potential of \approx 2.9 V (vs Na/Na^+) for SIBs. In addition, the fast Na^- ion transport in the P2-type $Na_{0.55}[N_{0.1}Fe_{0.1}Mn_{0.8}]O_2$ cathode structure enables good power capability with an extremely high current density of 2400 mA g^{-1} and long-term cycling stability with \approx 80% capacity retention after 500 cycles at 600 mA g^{-1} . A combination of electrochemical profiles, in operando synchrotron X-ray diffraction analysis, and first-principles calculations are used to understand the overall Na storage mechanism of P2-type $Na_{0.55}[N_{0.1}Fe_{0.1}Mn_{0.8}]O_2$.