$Na_3V(PO_3)_3N$: New zero-strain and 4V cathode material for Na-ion batteries

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These We developed $Na_3V(PO_3)_3N$ as a novel 4V-class and zero-strain cathode material for Na-ion batteries. Through the combined studies using neutron and X-ray diffraction, it was identified that the $Na_3V(PO_3)_3N$ contains 3-dimensional channels, which enables the facile Na diffusion in the structure. The Na (de)intercalation of $Na_3V(PO_3)_3N$ was occur at ~4 V (*vs.* Na/Na^+) via the V^{3+}/V^{4+} redox reaction and its capacity retention over 3000 cycles was ~67% of the initial capacity. The remarkable cycle stability was due to the near-zero volume change (~0.24%) and the unique centrosymmetric distortion that occurs during a cycle despite the large ionic size of Na ions for (de)intercalation, as demonstrated by ex-situ XRD analyses and first-principles calculations. We also demonstrated that the $Na_3V(PO_3)_3N$ could show the outstanding power capability with ~84% retention of the theoretical capacity at 10C, which is attributed to its intrinsic 3-dimensional open-crystal framework. The combination of this high power capability and extraordinary cycle stability enables the application of $Na_3V(PO_3)_3N$ to a promising cathode material for Na-ion batteries [1].

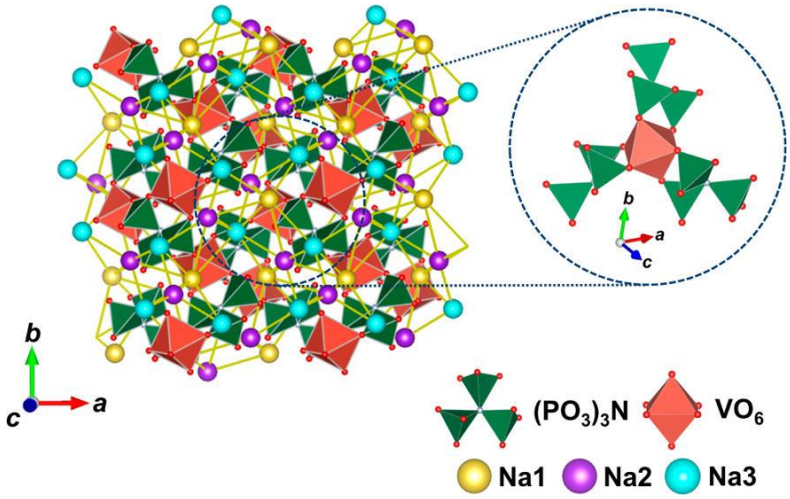

Fig. 6 Crystal structure of $Na_3V(PO_3)_3N$ [1].

[1] J. Kim *et al*, *Chem. Mater.* 29, 7826−7832 (2017)