

pH-regulative synthesis of $\text{Na}_3(\text{VPO}_4)_2\text{F}_3$ nanoflowers and their improved Na cycling stability

Yuruo Qi^{a,b}, Linqin Mu^c, Junmei Zhao^{a*}, Yong-Sheng Hu^{b,c}, Huizhou Liu^{a*}, Sheng Dai^d

^a Key Laboratory of Green Process and Engineering, Institute of Process Engineering, Chinese Academy of Sciences, Beijing 100190, China. Tel: +86-10-82544911. *E-mail: jmzhao@ipe.ac.cn

^b University of Chinese Academy of Sciences, Beijing 100049, PR China

^c Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

^d Chemical Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA

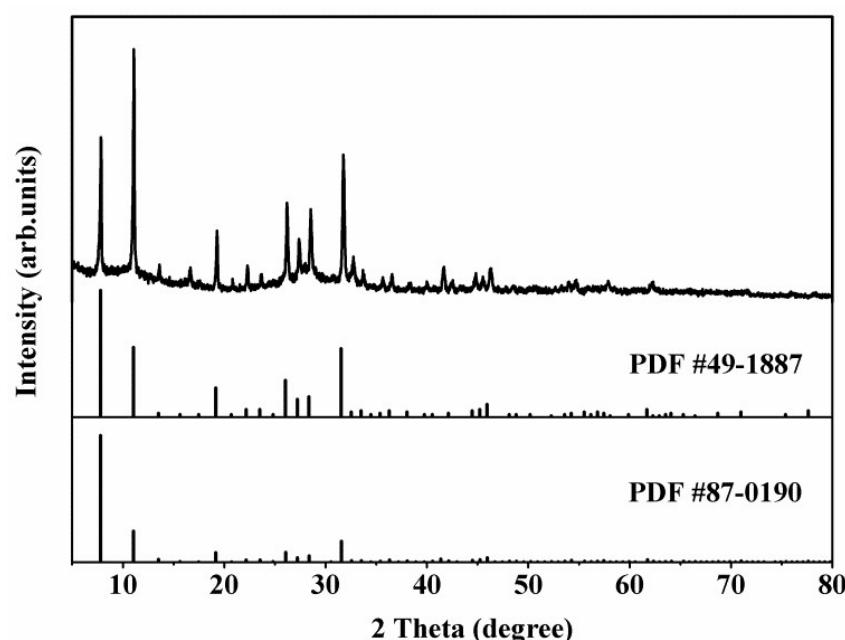
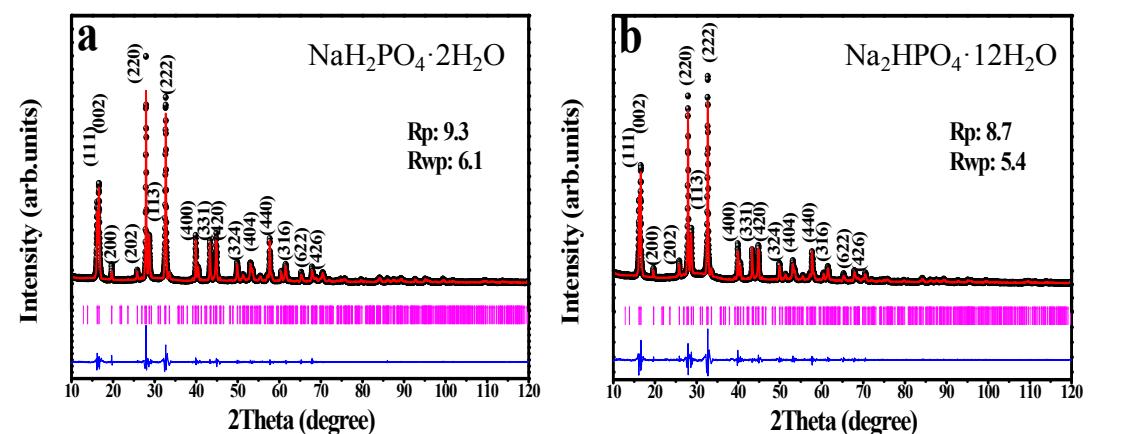


Fig. S1 XRD patterns of the solid product derived from Na_3PO_4 as phosphorus source,

JCPDS card # 49-1887 ($\text{Na}_{3.44}[(\text{V}_5\text{O}_9)(\text{PO}_4)_2](\text{PO}_4)_{0.08}(\text{OH})_{0.2}\cdot 9\text{H}_2\text{O}$) and # 87-0190 ($\text{Na}_{3.053}((\text{V}_5\text{O}_9)(\text{PO}_4)_2)(\text{OH})_{0.1}\cdot 8\text{H}_2\text{O}$).



	$\text{NaH}_2\text{PO}_4\cdot 2\text{H}_2\text{O}$	$\text{Na}_2\text{HPO}_4\cdot 12\text{H}_2\text{O}$
$a(\text{\AA})$	9.03535(7)	9.03181(6)
$b(\text{\AA})$	9.03535(7)	9.03181(6)
$c(\text{\AA})$	10.69549(6)	10.68671(6)
$V(\text{\AA}^3)$	873.2	871.8
Space Group	P42/mnm	P42/mnm
Crystal System	Tetragonal	Tetragonal

Fig. S2 The fitted profiles of $\text{Na}_3(\text{VPO}_4)_2\text{F}_3$ prepared by $\text{NaH}_2\text{PO}_4 \cdot 2\text{H}_2\text{O}$ (a) and $\text{Na}_2\text{HPO}_4 \cdot 12\text{H}_2\text{O}$ (b) and the corresponding fitted lattice parameters. The black (red) line represents the experimental (calculated) data. The residual discrepancy is shown in blue.

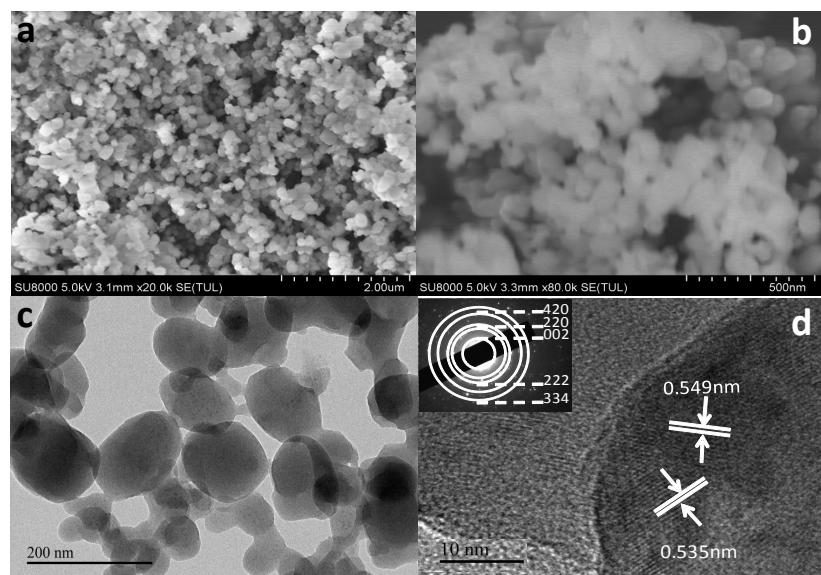


Fig. S3 Typical SEM images at the different magnifications (a-c), typical high-magnification TEM (HRTEM) image and corresponding SAED pattern (d) for $\text{Na}_3(\text{VPO}_4)_2\text{F}_3$ nanoparticles using $\text{Na}_2\text{HPO}_4 \square 12\text{H}_2\text{O}$ as phosphorus source.

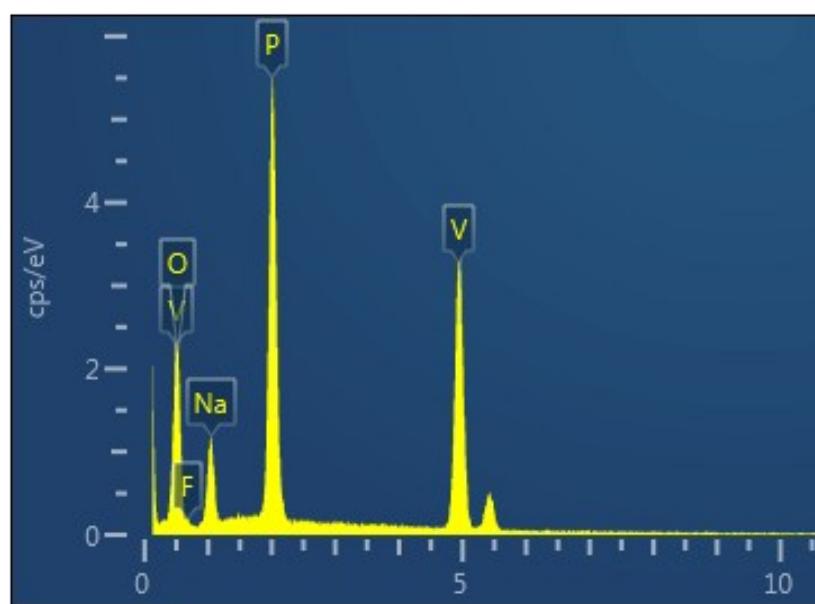


Fig. S4 EDS analysis of the product at 0 h taking $\text{NaH}_2\text{PO}_4 \cdot 2\text{H}_2\text{O}$ as phosphorus source.

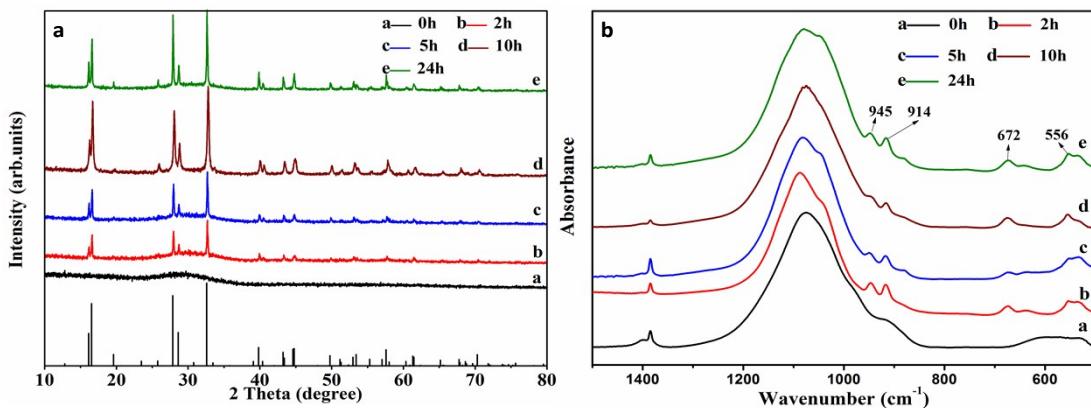


Fig. S5 (a) XRD patterns and (b) FTIR spectra of the products taking $\text{Na}_2\text{HPO}_4 \cdot 12\text{H}_2\text{O}$ as phosphorus source with a different hydro-thermal time.

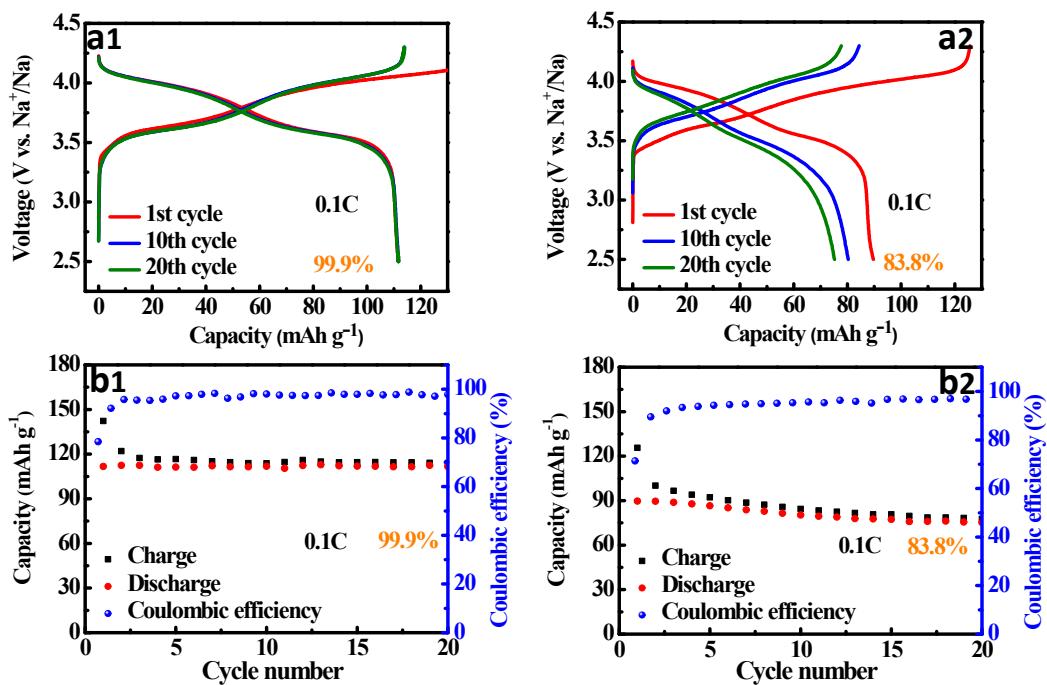


Fig. S6 Comparison of Na-storage properties between $\text{Na}_3(\text{VPO}_4)_2\text{F}_3$ nanoflower (1) prepared by $\text{NaH}_2\text{PO}_4 \square 2\text{H}_2\text{O}$ and $\text{Na}_3(\text{VPO}_4)_2\text{F}_3$ nanoparticles (2) prepared by $\text{Na}_2\text{HPO}_4 \cdot 12\text{H}_2\text{O}$. Galvanostatic charge and discharge curves (a); The cycling performance and Coulombic efficiency at a current rate of 0.1C (b).

