

Supporting information

Building High Power Density of Sodium-Ion Batteries: Importance of Multidimensional Diffusion Pathways in Cathode Materials

Mingzhe Chen, Yanyan Zhang, Guichuan Xing, Yuxin Tang*

¹Institute of Applied Physics and Materials Engineering, University of Macau, Macau, P. R. China

*** Correspondence:** yxtang@um.edu.mo

Keywords: high power density, multidimensional diffusion pathways, cathode materials, sodium-ion batteries devices, materials design

Table S1 Summary of kinetics parameters of reported 3D sodium diffusion cathodes for SIB devices.

Materials	Average Operation Voltage	Achievable Capacity (mAh g ⁻¹)	Rate Performance (mAh g ⁻¹)	Initial Coulombic Efficiency	Na ⁺ Diffusion - (cm ² s ⁻¹)	Highest Activation barrier	Volume Expansion	Reference
Fe ₄ [Fe(CN) ₆] ₃	3.4 V	68 (10 mA g ⁻¹)	59 (480 mA g ⁻¹)	-	-	-	0.72 %	(Ji et al., 2016)
Na ₂ FeFe(CN) ₆	2.9 V	170 (0.1 C)	120 (6 C)	90 %	10 ⁻¹⁰ –10 ⁻¹¹	0.64 eV	-	(You et al., 2016)
Na ₂ Mn[Mn(CN) ₆]	2.6 V	209 (40 mA g ⁻¹)	157 (1 A g ⁻¹)	99.5 %	-	-	1.36 %	(Lee et al., 2014)
Na ₂ Mn[Fe(CN) ₆]·zH ₂ O	3.4 V	150 (14.3 mA g ⁻¹)	122 (2.86 A g ⁻¹)	87 %	-	-	-	(Song et al., 2015)
Na _{1.68} Ni _{0.3} Co _{0.7} [Fe(CN) ₆]	3.3 V	143 (30 mA g ⁻¹)	88 (1.5 A g ⁻¹)	97 %	-	0.57 eV	3 %	(Peng et al., 2018)
Na ₄ Fe ₃ (PO ₄) ₂ (P ₂ O ₇)	3.2 V	113 (12 mA g ⁻¹)	80 (2.4 A g ⁻¹)	99 %	10 ⁻¹⁰ –10 ⁻¹³	0.82 eV	4.0 %	(Chen et al., 2019)

Na₃V(PO₃)₃N	4.0 V	73 (14.6 mA g ⁻¹)	62 (0.73 A g ⁻¹)	-	-	0.8 eV	0.24 %	(Kim et al., 2017)
Na₄Mn₃(PO₄)₂(P₂O₇)	3.8 V	109 (0.05 C)	55 (20 C)	88 %	-	0.56 eV	7.0 %	(Kim et al., 2015)
Na₃V₂(PO₄)₃	-	-	-	-	10 ⁻¹⁰ –10 ⁻¹²	0.6 eV	-	(Bui et al., 2015)
Na₃V₂(PO₄)₃	3.3 V	113 (0.5 C)	90 (10 C)	-	10 ⁻¹¹ –10 ⁻¹²	0.395 eV	7.6 %	(Li et al., 2018)
Na₃MnZr(PO₄)₃	3.8 V	107 (0.1 C)	50 (20 C)	87 %	-	-	5.5 %	(Gao et al., 2018)
Na₃MnTi(PO₄)₃	2.5 V	162 (0.2 C)	130 (2 C)	155 %	10 ⁻¹¹ –10 ⁻¹³	-	-	(Zhu et al., 2019)

References

- Bui, K.M., Dinh, V.A., Okada, S., and Ohno, T. (2015). Hybrid functional study of the NASICON-type $\text{Na}_3\text{V}_2(\text{PO}_4)_3$: crystal and electronic structures, and polaron-Na vacancy complex diffusion. *Phys. Chem. Chem. Phys.* 17(45), 30433-30439. doi: 10.1039/c5cp05323d
- Chen, M., Hua, W., Xiao, J., Cortie, D., Chen, W., Wang, E., et al. (2019). NASICON-type air-stable and all-climate cathode for sodium-ion batteries with low cost and high-power density. *Nat. Commun.* 10(1), 1480. doi: 10.1038/s41467-019-09170-5
- Gao, H., Seymour, I. D., Xin, S., Xue, L., Henkelman, G., and Goodenough, J.B. (2018). $\text{Na}_3\text{MnZr}(\text{PO}_4)_3$: A High-Voltage Cathode for Sodium Batteries. *J. Am. Chem. Soc.* 140(51), 18192-18199. doi: 10.1021/jacs.8b11388
- Ji, Z., Han, B., Liang, H., Zhou, C., Gao, Q., Xia, K., et al. (2016). On the Mechanism of the Improved Operation Voltage of Rhombohedral Nickel Hexacyanoferrate as Cathodes for Sodium-Ion Batteries. *ACS Appl. Mater. Interfaces* 8(49), 33619-33625. doi: 10.1021/acsami.6b11070
- Kim, H., Yoon, G., Park, I., Park, K.-Y., Lee, B., Kim, J., et al. (2015). Anomalous Jahn–Teller behavior in a manganese-based mixed-phosphate cathode for sodium ion batteries. *Energy Environ. Sci.* 8(11), 3325-3335. doi: 10.1039/c5ee01876e
- Kim, J., Yoon, G., Lee, M.H., Kim, H., Lee, S., and Kang, K. (2017). New 4V-Class and Zero-Strain Cathode Material for Na-Ion Batteries. *Chem. Mater.* 29(18), 7826-7832. doi: 10.1021/acs.chemmater.7b02477
- Lee, H.-W., Wang, R.Y., Pasta, M., Lee, S.W., Liu, N., and Cui, Y. (2014). Manganese hexacyanomanganate open framework as a high-capacity positive electrode material for sodium-ion batteries. *Nat. Commun.* 5, 5280. doi: 10.1038/ncomms6280
- Li, X., Huang, Y., Wang, J., Miao, L., Li, Y., Liu, Y., et al. (2018). High valence Mo-doped $\text{Na}_3\text{V}_2(\text{PO}_4)_3/\text{C}$ as a high rate and stable cycle-life cathode for sodium battery. *J. Mater. Chem. A* 6(4), 1390-1396. doi: 10.1039/c7ta08970h
- Peng, J., Wang, J., Yi, H., Hu, W., Yu, Y., Yin, J., et al. (2018). A Dual-Insertion Type Sodium-Ion Full Cell Based on High-Quality Ternary-Metal Prussian Blue Analogs. *Adv. Energy Mater.* 8(11), 1702856. doi: 10.1002/aenm.201702856
- Song, J., Wang, L., Lu, Y., Liu, J., Guo, B., Xiao, P., et al. (2015). Removal of Interstitial H_2O in Hexacyanometallates for A Superior Cathode of A Sodium-ion Battery. *J Am. Chem. Soc.* 137(7), 2658-2664. doi: 10.1021/ja512383b
- You, Y., Yao, H.R., Xin, S., Yin, Y.X., Zuo, T. T., Yang, C.P., et al. (2016). Subzero-Temperature Cathode for a Sodium-Ion Battery. *Adv. Mater.* 28(33), 7243-7248. doi: 10.1002/adma.201600846

Zhu, T., Hu, P., Wang, X., Liu, Z., Luo, W., Owusu, K.A., et al. (2019). Realizing Three-Electron Redox Reactions in NASICON-Structured $\text{Na}_3\text{MnTi}(\text{PO}_4)_3$ for Sodium-Ion Batteries. *Adv. Energy Mater.* 9(9), 1803436. doi: 10.1002/aenm.201803436