Supporting information

Single-crystalline Mg-substituted $Na_4Mn_3(PO_4)_2P_2O_7$ nanoparticles as high capacity and superior cycling cathode of sodium-ion batteries

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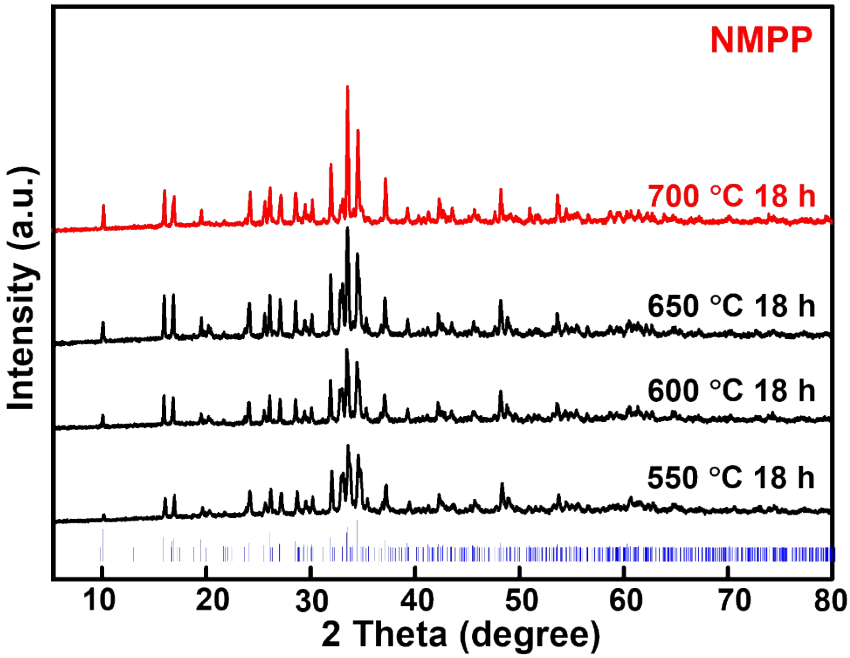

Fig. S1 XRD patterns of prepared NMPP at different temperatures.

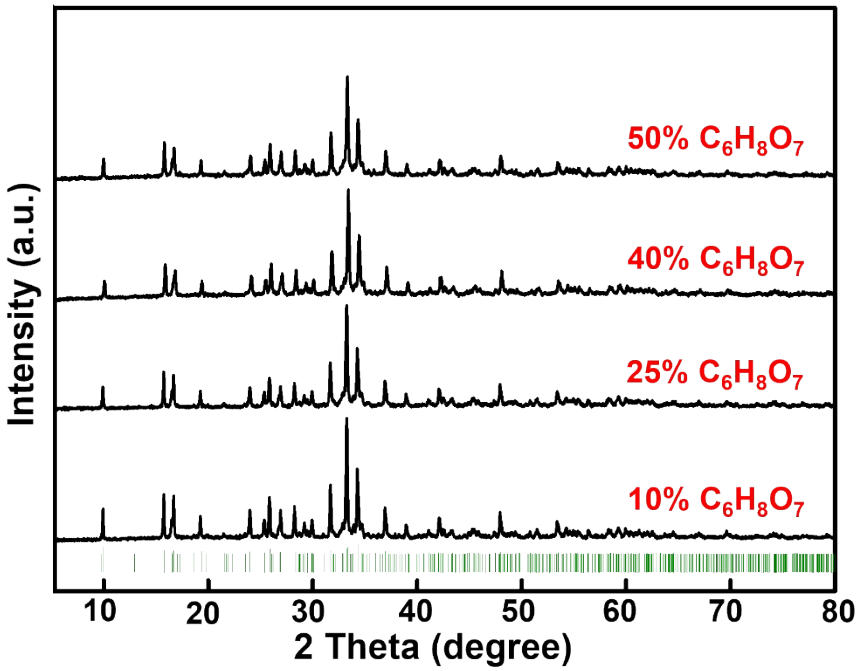

Fig. S2 XRD patterns of prepared NMPP@C composites at different carbon-coated proportions.

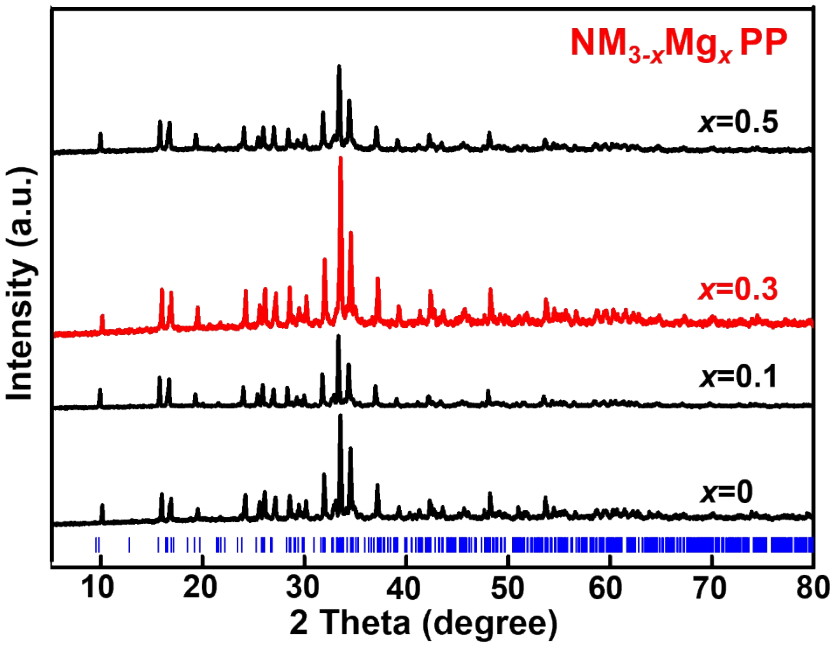

Fig. S3 XRD patterns of prepared $NM_{3-x}Mg_xPP$@C composites with different Mg substitution proportions.

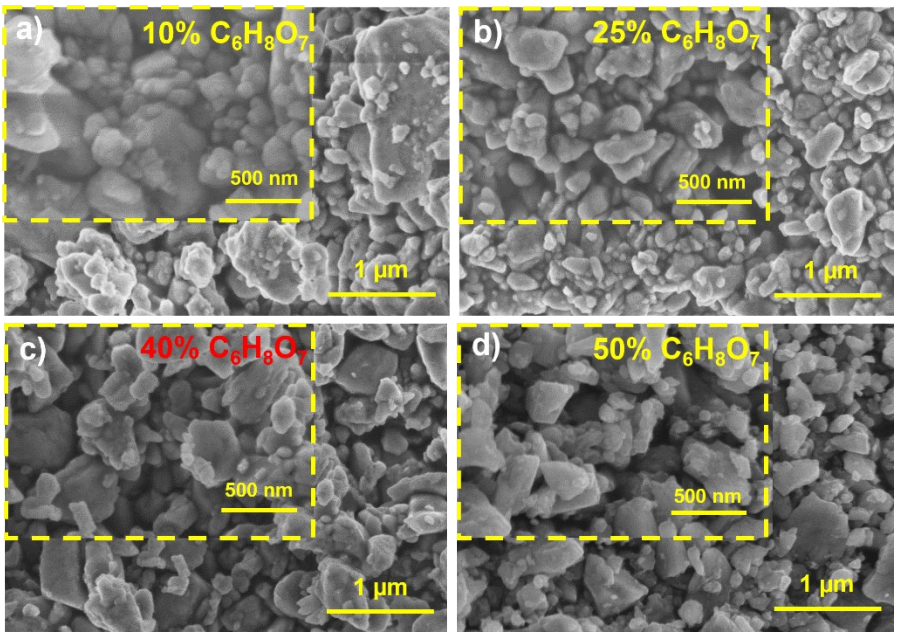

Fig. S4 SEM images of NMPP@C composites prepared by the different $C_6H_8O_7$ precursors.

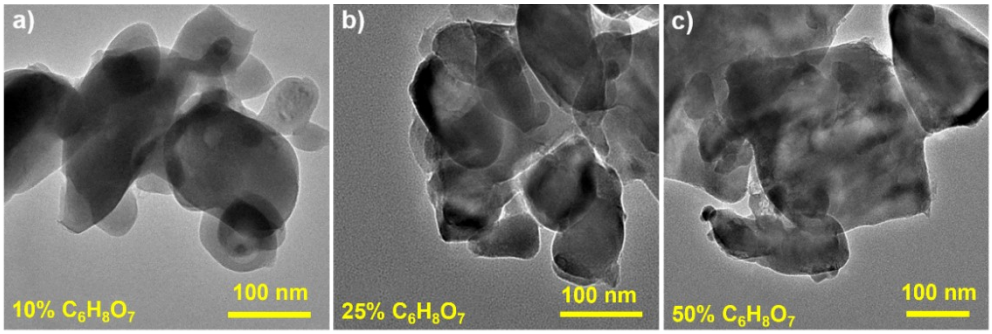

Fig. S5 TEM images of NMPP@C composites prepared by the different $C_6H_8O_7$ precursors.

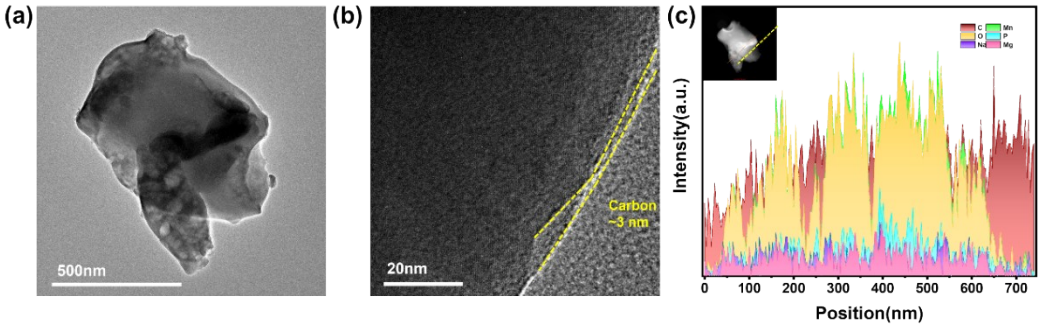

Figure S6. STEM and STEM line-scan images of $NM_{2.7}Mg_{0.3}PP@C$ samples.

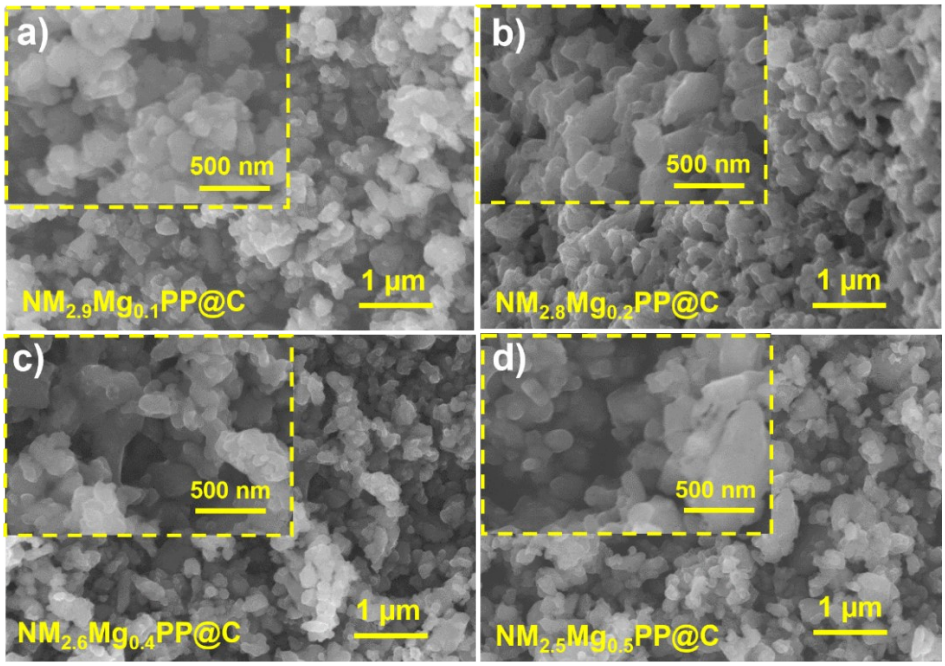

Fig. S7 SEM images of $NM_{3-x}Mg_xPP@C$ composites with different Mg substitution proportions.

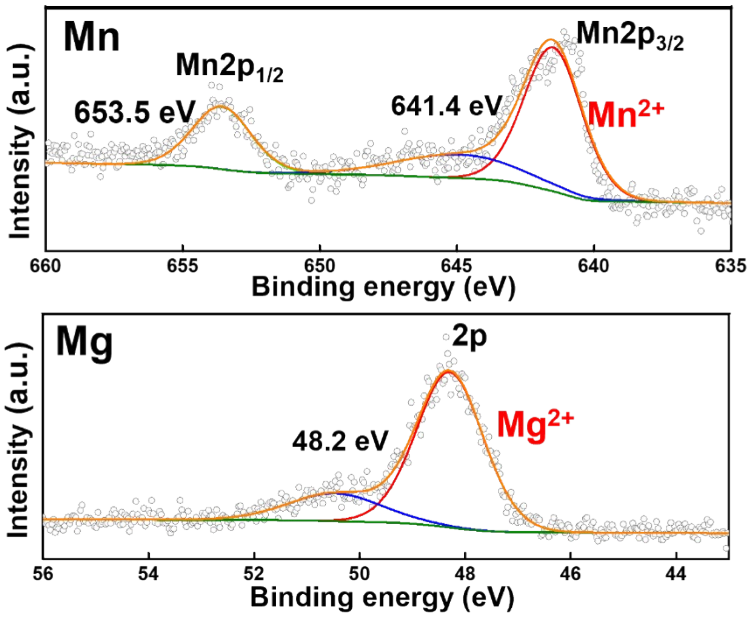

Fig. S8 XPS spectra of $NM_{2.7}Mg_{0.3}PP$@C sample.

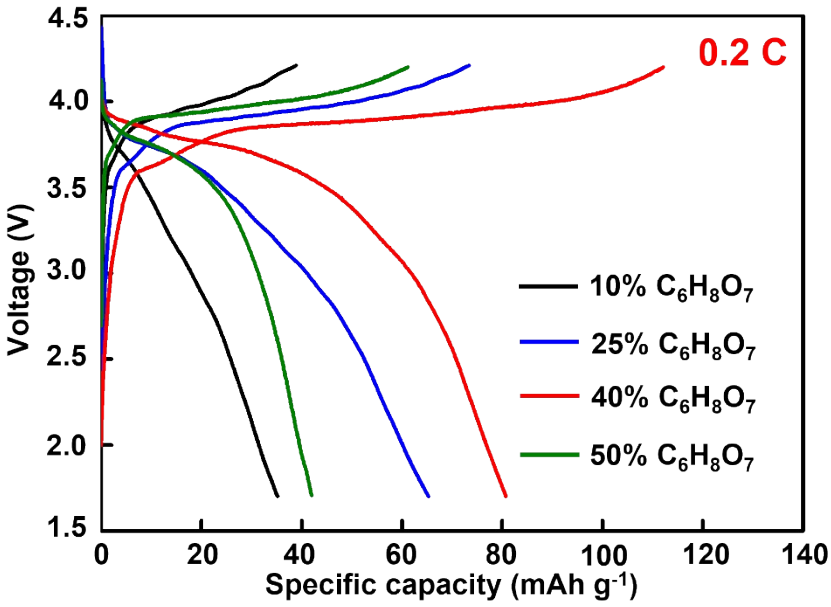

Fig. S9 Charge/discharge curves of NMPP@C cathodes at 0.2 C.

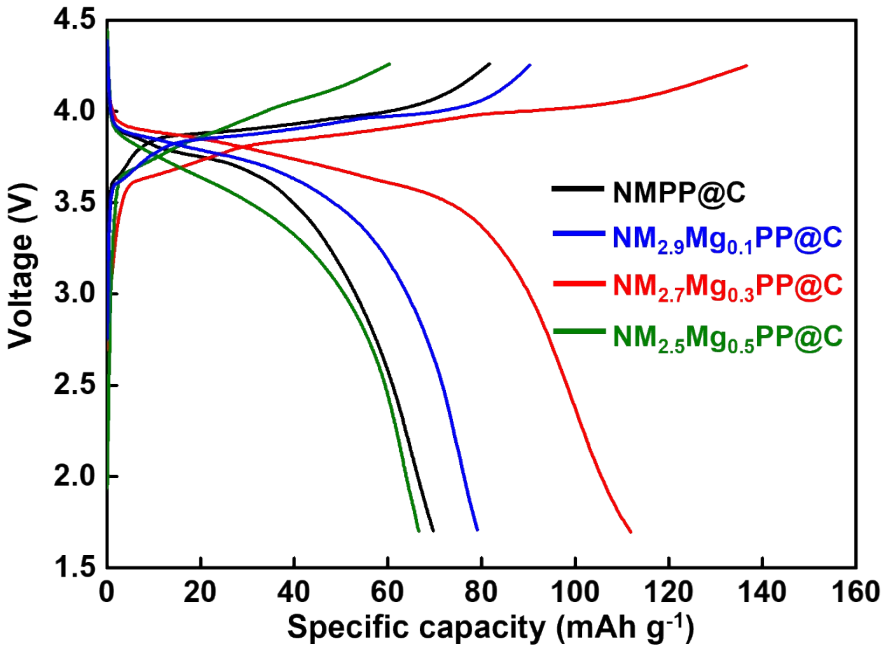

Fig. S10 Charge/discharge curves of $NM_{3-x}Mg_xPP@C$ cathodes at 0.2 C.

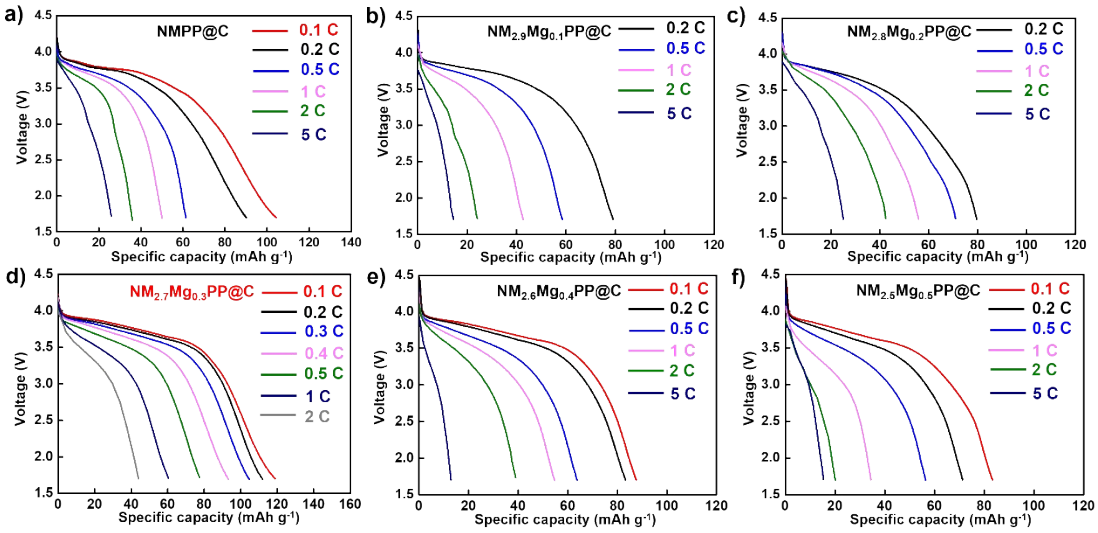

Fig. S11 Charge/discharge curves of $NM_{3-x}Mg_xPP@C$ cathodes at different current densities.

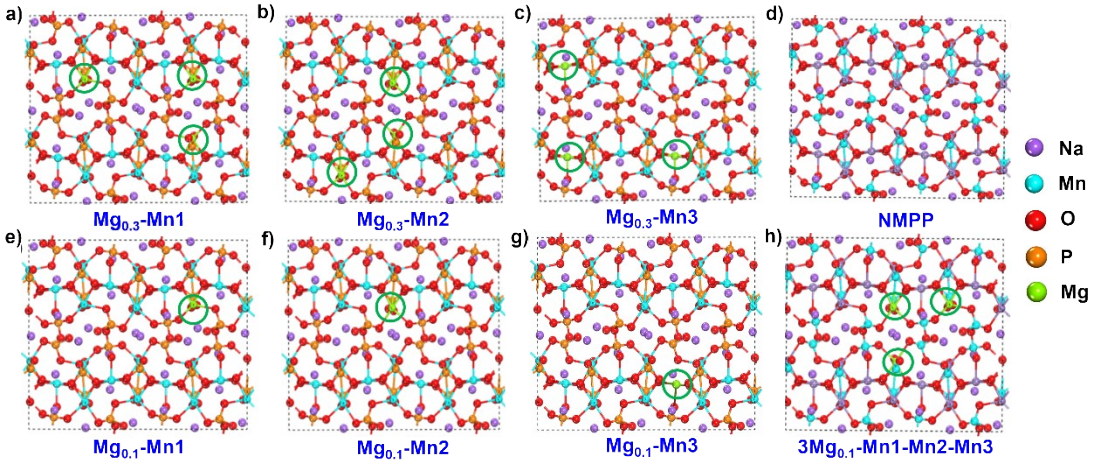

Fig. S12 Crystal structure models based on various Mg-substituted sites.

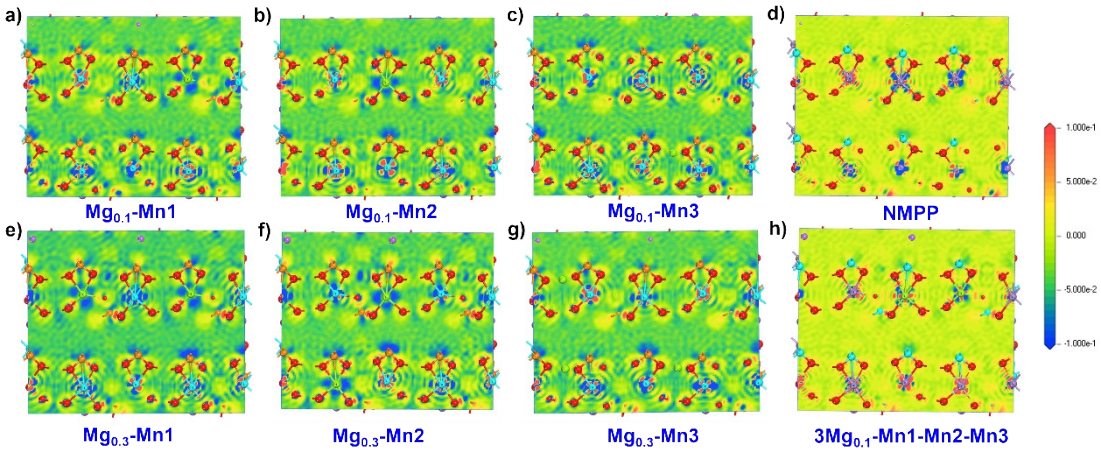

Fig. S13 Charge density diagrams of different crystal models based on various Mg-substituted sites.

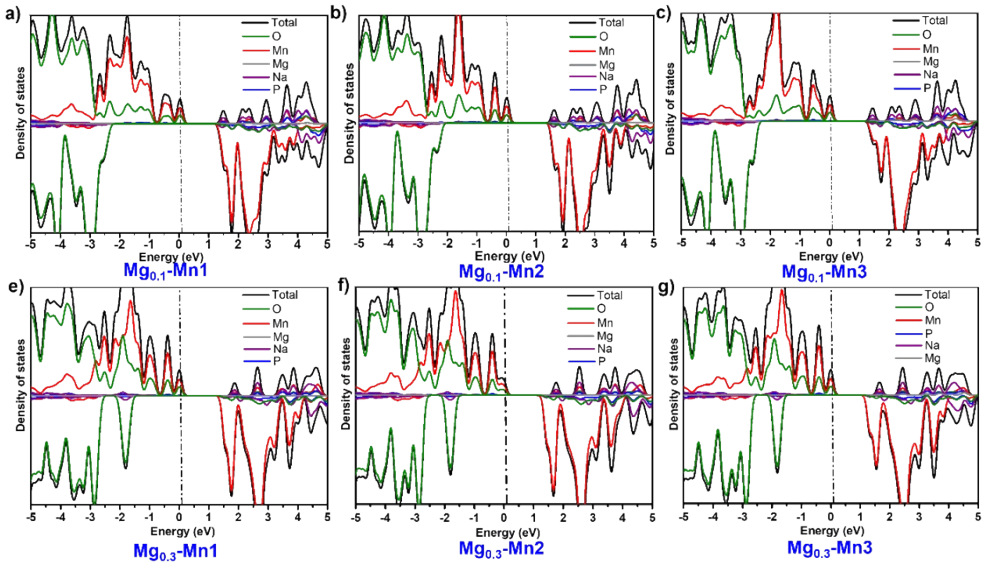

Fig. S14 DOS curves of different crystal models based on various Mg-substituted sites.

TableS1 Rietveld XRD refinements results of NMPP@C and $NM_{2.7}Mg_{0.3}PP$@C samples

Chemical formula	$Na_4Mn_3(PO_4)_2P_2O_7$@C	$Na_4Mn_{2.7}Mg_{0.3}(PO_4)_2P_2O_7$@C
Space group	P n 2_1 a(No.33)	
a(Å)	17.9773 (9)	17.9471 (9)
b(Å)	6.6357 (3)	6.6272 (4)
c(Å)	10.7652	10.7620 (6)
V(Å^3)	1282.05 (9)	1278.20 (12)
$R_p/R_{wp}/R_{exp}$	2.18/3.27/1.40	2.28/3.25/2.04

Table S2 Fractional coordinates and site occupancies of Mg and Mn in refined XRD pattern of $NM_{2.7}Mg_{0.3}PP$ material

atom	x	y	z	Occ.
Mn1	0.34016	0.09090	0.50140	0.900
Mn2	0.14287	0.60340	0.48490	0.900
Mn3	0.23901	0.32540	0.75260	0.900
Mg1	0.34016	0.09090	0.50140	0.100
Mg2	0.14287	0.60340	0.48490	0.100
Mg3	0.23901	0.32540	0.75260	0.100