Electronic Supplementary Material (ESI) for RSC Advances.

Electronic supplementary information (ESI)

Superior high rate capability of size-controlled $LiMnPO_4$/C nanosheets with preferential orientation

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Table S1. The final atomic coordinates, isotropic temperature factors, and agreement factors of (a) M1/DBSA/S and (b) M2/DBSA/S, respectively.

(a) $LiMnPO_4$ (M1/DBSA/S)			R_p = 10.0%, R_{wp} = 14.3%, R_{exp} = 14.86%, χ^2 = 0.922				
	Atom	Site	g	x	y	z	B_{iso}
Pnma	Li	4a	0.50	0	0	0	2.449 (14)
$Mn^{\bullet}_{Li}$% = 0.04	Mn	4c	0.50	0.280 (39))	0.250 (00)	0.979 (11)	2.449 (14)
a = 10.440 Å	P	4c	0.50	0.099 (80)	0.250 (00)	0.415 (15)	1.826 (214)
b = 6.102 Å	O	4c	0.50	0.097 (133)	0.250 (00)	0.726 (249)	2.656 (218)
c = 4.757 Å	O	4c	0.50	0.320 (689)	0.250 (00)	0.281 (209)	2.620 (999)
	O	8d	1.00	0.186 (247)	0.023 (24)	0.305 (242)	2.254 (392)

(b) $LiMnPO_4$ (M2/DBSA/S)			R_p = 9.3%, R_{wp} = 12.2%, R_{exp} = 9.58%, χ^2 = 1.02				
	Atom	Site	g	x	y	z	B_{iso}
Pnma	Li	4a	0.50	0	0	0	2.451 (52)
$Mn^{\bullet}_{Li}$% = 0.02	Mn	4c	0.50	0.280 (57))	0.250 (00)	0.968 (46)	2.451 (52)
a = 10.443 Å	P	4c	0.50	0.095 (56)	0.250 (00)	0.405 (79)	1.756 (45)
b = 6.095 Å	O	4c	0.50	0.095 (45)	0.250 (00)	0.727 (54)	1.636 (105)
c = 4.752 Å	O	4c	0.50	0.456 (38)	0.250 (00)	0.225 (149)	1.636 (105)
	O	8d	1.00	0.169 (54)	0.047 (87)	0.280 (99)	1.636 (105)

Table S2. Migration energies of Li ion in $LiMnPO_4$

Migration path	[010]	[101]	[001]
E_{mig} (eV)	0.62	2.26	2.83

Table S3. The final atomic coordinates, isotropic temperature factors, and agreement factors of M2/P123/S.

$LiMnPO_4$ (M2/P123/S)			R_p = 10.1%, R_{wp} = 12.3%, R_{exp} = 9.65%, χ^2 = 0.983				
	Atom	Site	g	x	y	z	B_{iso}
Pnma	Li	4a	0.50	0	0	0	2.431 (54)
$Mn^{\bullet}_{Li}$% = 0.014	Mn	4c	0.50	0.281 (26))	0.250 (00)	0.966 (25)	2.431 (54)
a = 10.443 Å	P	4c	0.50	0.090 (54)	0.250 (00)	0.403 (89)	1.920 (66)
b = 6.099 Å	O	4c	0.50	0.095 (12)	0.250 (00)	0.732 (53)	0.705 (105)
c = 4.755 Å	O	4c	0.50	0.451 (83)	0.250 (00)	0.206 (133)	2.318 (194)
	O	8d	1.00	0.162 (63)	0.047 (98)	0.276 (98)	2.385 (102)

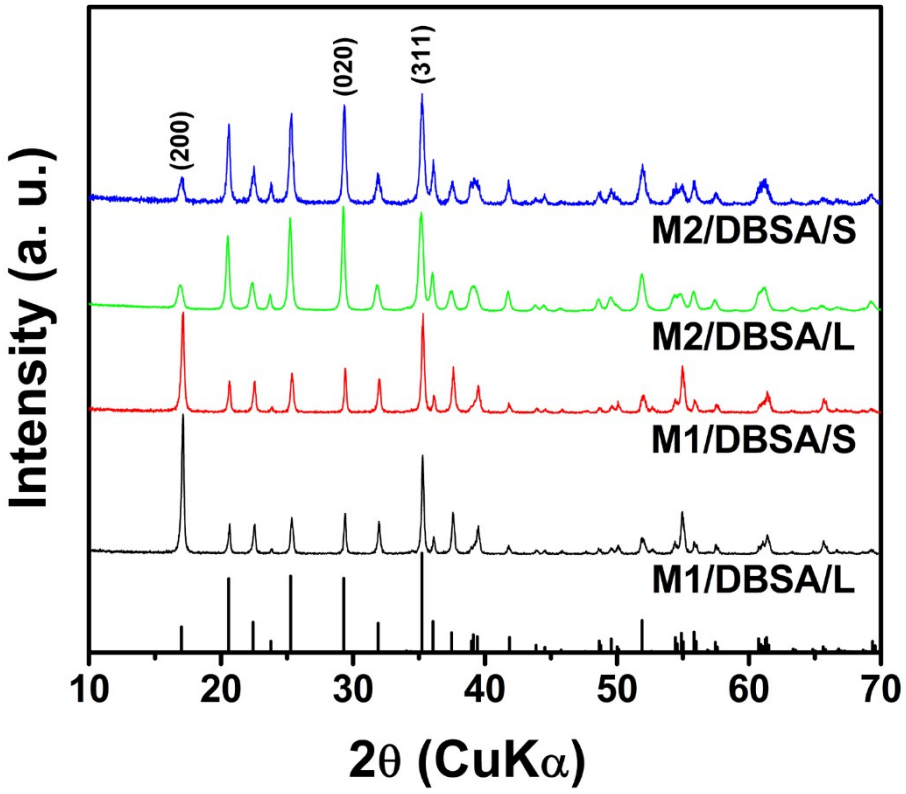

Fig. S1. XRD patterns of (a) M1/DBSA/L, (b) M1/DBSA/S, (c) M2/DBSA/L and (d) M2/DBSA/S.

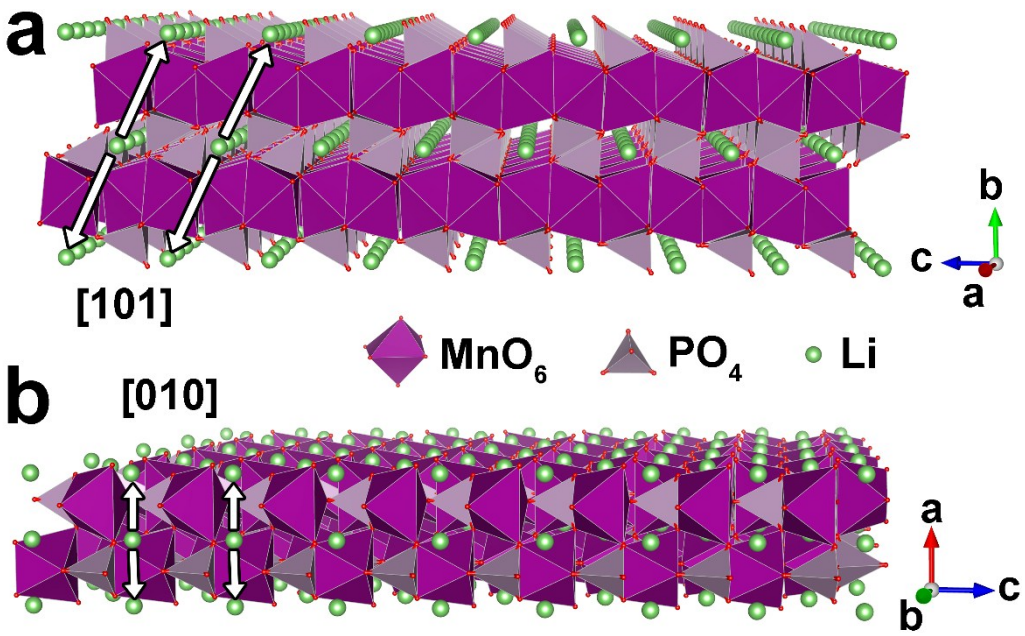

Fig. S2. Paths considered for Li ion migration in $LiMnPO_4$. The preferred facet orientation is (a) {100} plane and (b) {010} plane.

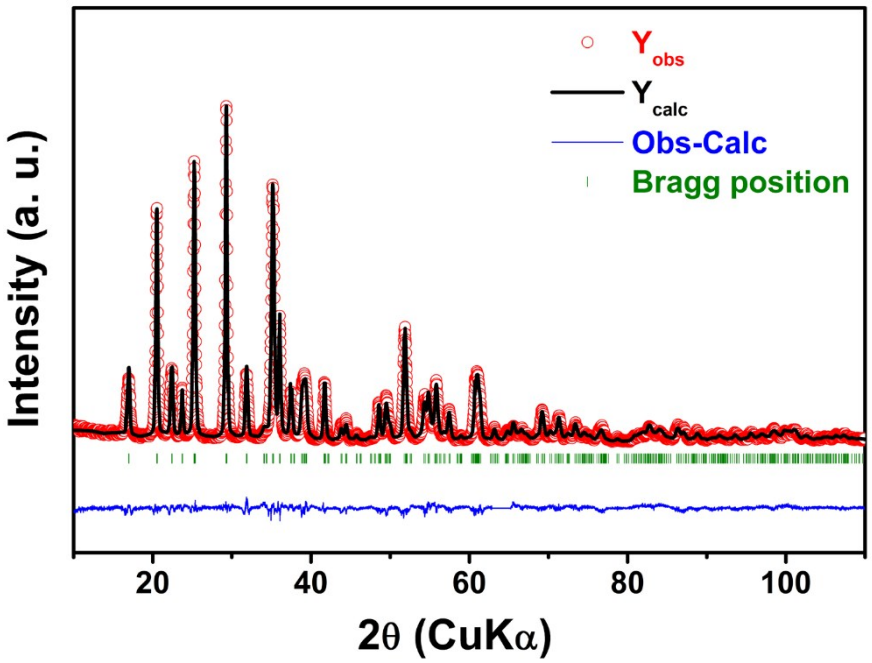

Fig. S3. Rietveld refinement of M2/P123/S. The black solid curve is the calculated diffraction data, the red "○" marks are the observed diffraction data, and the olivine straight bars are the Bragg positions of the simulated diffraction patterns. The deviation between the calculated and the observed value is represented by the blue solid line beneath the curves.