

Electronic Supplementary Information

Ionothermal synthesis of a three-dimensional manganese(II) phosphate with zeolite DFT topology

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All chemicals used during this investigation were reagent grade. They were used as received. Elemental analyses of C, H and N were carried out with a Perkin-Elmer 2400 elemental analyzer. Inductively coupled plasma (ICP) analysis was performed on a Perkin-Elmer Optima 3300DV spectrometer. X-ray powder diffraction (XRD) data were collected on a Rigaku D-Max 2550 diffractometer with Cu K α radiation ($\lambda = 1.5418\text{\AA}$). The morphology and EDS analysis of the crystals were observed on field emission scanning electron microscope (SEM, Hitachi, S-4300). Thermogravimetric analysis (TGA) was carried out on a TGA Q500 system in air with a heating rate of 10 K min⁻¹. The X-ray photoelectron spectra (XPS) were recorded on a VG ESCALAB MK II electron spectrometer. Temperature dependent magnetic susceptibility data were recorded on a Quantum-Design MPMS-XL SQUID magnetometer under an applied field of 1000 Oe over the temperature range of 2-300 K.

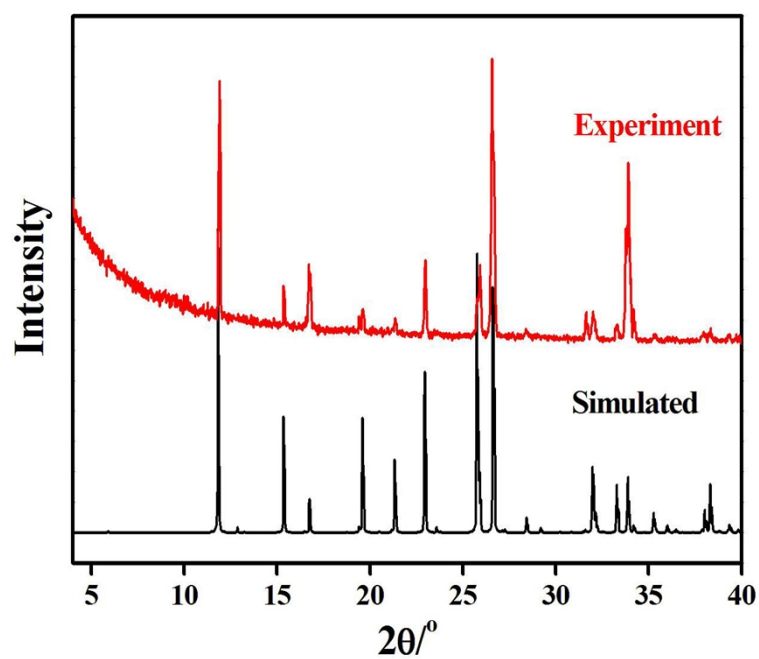


Fig. S1 Simulated (black) and experimental XRPD patterns of JIS-14 (red)

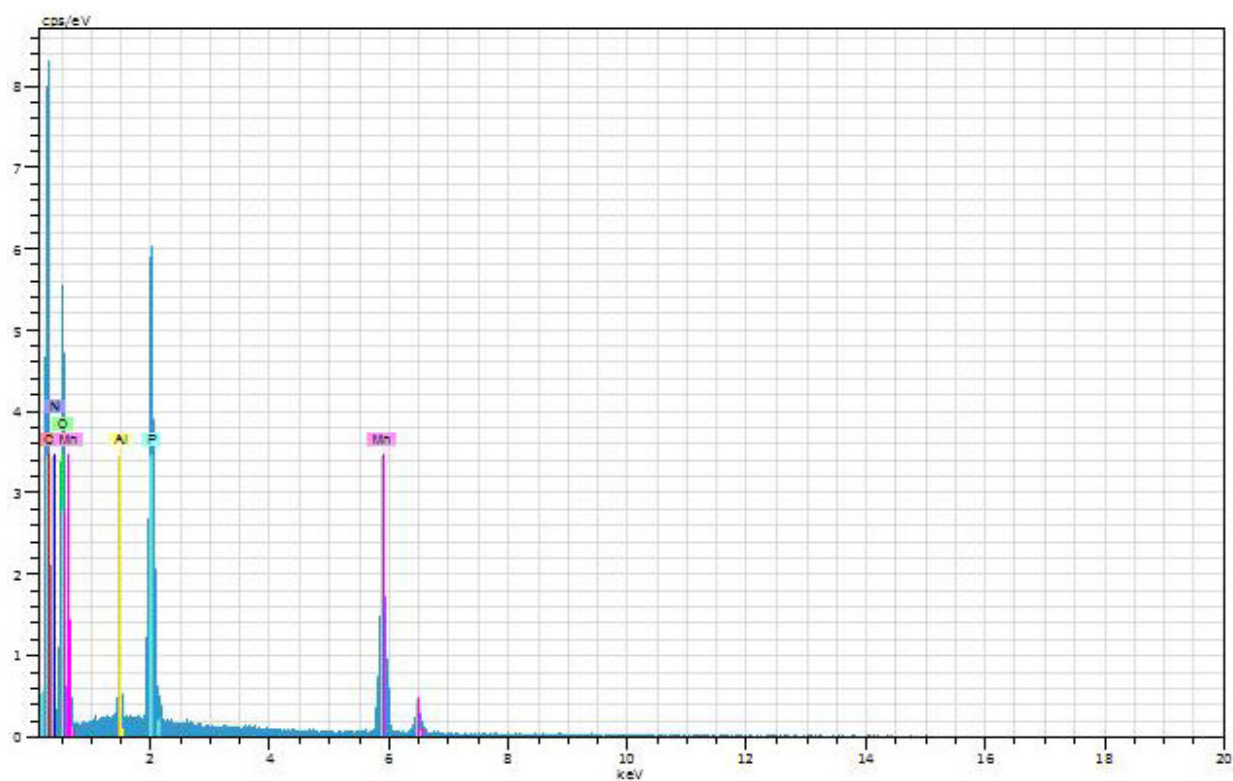


Fig. S2 EDS spectra of JIS-14

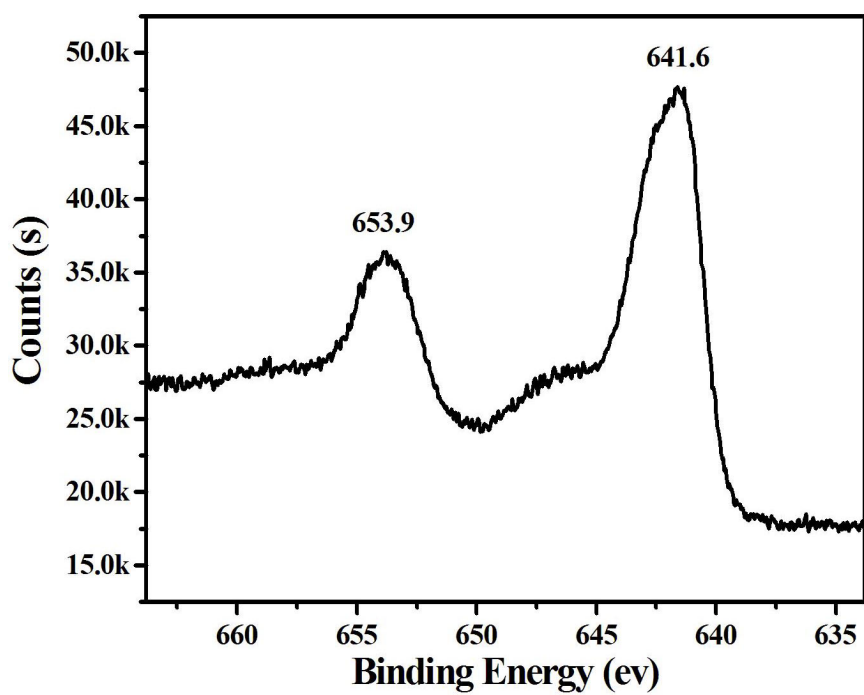


Fig. S3 XPS spectrum of JIS-14;

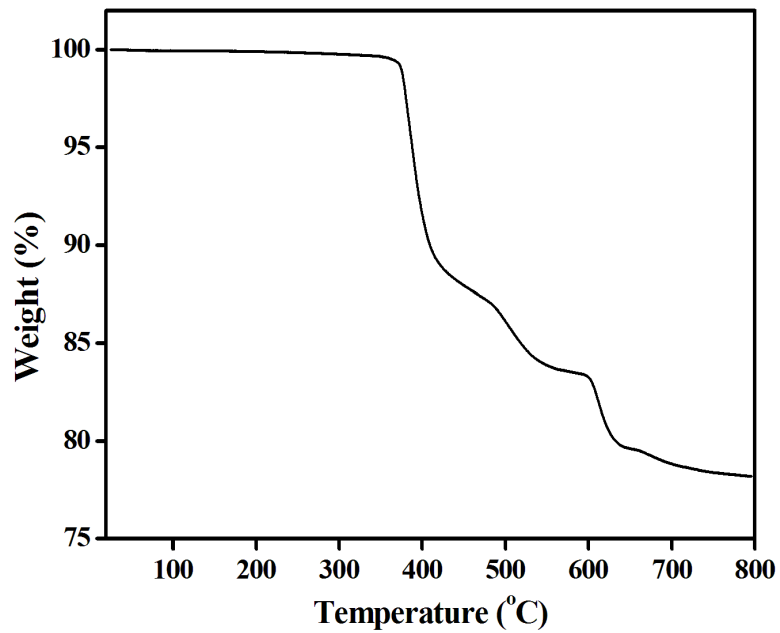


Fig. S4 TGA curve of JIS-14

Table S1 Selected Bond lengths [Å] and bond angles [deg.] for JIS-14

Mn(1)-O(2)#1	2.004(4)	P(1)-O(2)	1.514(4)
Mn(1)-O(1)	2.014(3)	P(1)-O(3)	1.516(5)
Mn(1)-O(3)#2	2.026(5)	P(1)-O(4)	1.525(4)
Mn(1)-O(5)	2.058(4)	P(1)-O(1)	1.540(4)
Mn(2)-O(8)#3	1.990(4)	P(2)-O(7)	1.523(4)
Mn(2)-O(13)	2.014(4)	P(2)-O(8)	1.524(5)
Mn(2)-O(9)	2.032(4)	P(2)-O(6)	1.525(4)
Mn(2)-O(6)	2.041(4)	P(2)-O(5)	1.534(4)
Mn(3)-O(12)#4	2.005(3)	P(3)-O(11)	1.522(6)
Mn(3)-O(11)#5	2.023(5)	P(3)-O(12)	1.526(4)
Mn(3)-O(15)#5	2.068(4)	P(3)-O(9)	1.531(4)
Mn(3)-O(10)	2.107(4)	P(3)-O(10)	1.531(4)
Mn(4)-O(14)#6	1.993(4)	P(4)-O(14)	1.514(5)
Mn(4)-O(7)#7	2.013(4)	P(4)-O(13)	1.522(4)
Mn(4)-O(4)	2.021(4)	P(4)-O(16)	1.526(4)
Mn(4)-O(16)#8	2.060(4)	P(4)-O(15)	1.538(4)
O(2)#1-Mn(1)-O(1)	114.90(17)	O(8)#3-Mn(2)-O(13)	114.9(2)
O(2)#1-Mn(1)-O(3)#2	109.0(2)	O(8)#3-Mn(2)-O(9)	106.0(2)
O(1)-Mn(1)-O(3)#2	118.92(17)	O(13)-Mn(2)-O(9)	109.69(19)
O(2)#1-Mn(1)-O(5)	97.11(17)	O(8)#3-Mn(2)-O(6)	114.6(2)
O(1)-Mn(1)-O(5)	105.36(15)	O(13)-Mn(2)-O(6)	113.69(17)
O(3)#2-Mn(1)-O(5)	109.07(18)	O(9)-Mn(2)-O(6)	95.88(19)
O(12)#4-Mn(3)-O(11)#5	110.34(18)	O(14)#6-Mn(4)-O(7)#7	112.6(2)
O(12)#4-Mn(3)-O(15)#5	105.64(17)	O(14)#6-Mn(4)-O(4)	107.6(2)
O(11)#5-Mn(3)-O(15)#5	109.07(19)	O(7)#7-Mn(4)-O(4)	106.80(18)
O(12)#4-Mn(3)-O(10)	119.58(16)	O(14)#6-Mn(4)-O(16)#8	123.0(2)
O(11)#5-Mn(3)-O(10)	113.3(2)	O(7)#7-Mn(4)-O(16)#8	108.51(19)
O(15)#5-Mn(3)-O(10)	97.38(18)	O(4)-Mn(4)-O(16)#8	96.03(18)
O(2)-P(1)-O(3)	111.5(3)	O(7)-P(2)-O(8)	111.0(3)
O(2)-P(1)-O(3)	108.8(2)	O(7)-P(2)-O(6)	111.7(3)
O(3)-P(1)-O(4)	111.1(3)	O(8)-P(2)-O(6)	111.1(3)
O(2)-P(1)-O(1)	110.3(2)	O(7)-P(2)-O(5)	111.2(3)
O(3)-P(1)-O(1)	107.5(2)	O(8)-P(2)-O(5)	103.9(3)
O(4)-P(1)-O(1)	107.5(2)	O(6)-P(2)-O(5)	107.7(2)
O(11)-P(3)-O(12)	111.1(2)	O(14)-P(4)-O(13)	110.1(3)
O(11)-P(3)-O(9)	110.0(3)	O(14)-P(4)-O(16)	110.1(3)
O(12)-P(3)-O(9)	106.1(2)	O(13)-P(4)-O(16)	112.3(3)
O(11)-P(3)-O(10)	113.5(3)	O(14)-P(4)-O(15)	104.2(3)
O(12)-P(3)-O(10)	107.3(2)	O(13)-P(4)-O(15)	110.7(3)
O(9)-P(3)-O(10)	108.5(2)	O(16)-P(4)-O(15)	109.2(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,z #2 -y+1,x,z+1/2 #3 -x+1,-y,z #4 -x+2,-y,z #5 y+1,-x+1,z+1/2 #6 y,-x+1,z+1/2
 #7 y,-x+1,z-1/2 #8 -y,x,z+1/2 #9 -y+1,x-1,z-1/2 #10 -y+1,x,z-1/2 #11 y,-x,z-1/2