Three isostructural MOFs based on different metal cations: proton conductivities and SC-SC transformation leading to magnetic changes

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Table S1 The selected bond lengths and angels of compounds **1-3** and **1**·CH_3OH.

1			
Co(1)-O(5)#1	1.998(3)	Co(1)-O(3)#2	2.043(3)
Co(1)-O(6)	2.216(4)	Co(1)-O(2)#2	2.270(3)
Co(1)-O(4)	2.013(3)	Co(1)-O(7)	2.104(3)
O(7)-Co(1)-O(6)	179.25(12)	O(4)-Co(1)-O(7)	88.00(14)
O(4)-Co(1)-O(6)	91.31(13)	O(6)-Co(1)-O(2)#2	94.82(12)
O(7)-Co(1)-O(2)#2	85.92(13)	O(5)#1-Co(1)-O(4)	109.43(13)
O(5)#1-Co(1)-O(4)	109.43(13)	O(5)#1-Co(1)-O(7)	91.67(14)
O(4)-Co(1)-O(3)#2	102.90(13)	O(5)#1-Co(1)-O(6)	88.29(14)
O(3)#2-Co(1)-O(7)	93.61(14)	O(5)#1-Co(1)-O(3)#2	147.39(14)
O(3)#2-Co(1)-O(6)	86.82(13)	O(5)#1-Co(1)-O(2)#2	88.05(12)
O(3)#2-Co(1)-O(2)#2	60.33(11)	O(4)-Co(1)-O(2)#2	161.67(12)
1·CH_3OH			
Co(1)-O(5)	2.018(4)	Co(1)-O(6)#1	2.025(5)
Co(1)-O(1)	2.103(6)	Co(1)-O(2)	2.112(6)
Co(1)-O(3)#2	2.129(5)	Co(1)-O(4)#2	2.220(4)
O(5)-Co(1)-O(1)	86.9(2)	O(5)-Co(1)-O(6)#1	116.2(2)
O(5)-Co(1)-O(2)	89.3(2)	O(6)#1-Co(1)-O(1)	84.2(2)
O(1)-Co(1)-O(2)	171.2(2)	O(6)#1-Co(1)-O(2)	90.5(2)
O(6)#1-Co(1)-O(3)#2	153.13(18)	O(5)-Co(1)-O(3)#2	90.72(18)
O(2)-Co(1)-O(3)#2	90.4(2)	O(1)-Co(1)-O(3)#2	97.5(2)
O(6)#1-Co(1)-O(4)#2	93.29(17)	O(5)-Co(1)-O(4)#2	150.03(19)
O(2)-Co(1)-O(4)#2	96.3(2)	O(1)-Co(1)-O(4)#2	91.0(2)
2			
Mn(1)-O(5)	2.053(11)	Mn(1)-O(2)#2	2.355(10)

Mn(1)-O(4)#1	2.118(9)	Mn(1)-O(7)	2.206(11)
Mn(1)-O(3)#2	2.184(9)	Mn(1)-O(6)	2.232(11)
O(5)-Mn(1)-O(3)#2	97.9(4)	O(5)-Mn(1)-O(4)#1	117.9(4)
O(4)#1-Mn(1)-O(3)#2	144.2(4)	O(4)#1-Mn(1)-O(7)	86.9(4)
O(5)-Mn(1)-O(7)	88.5(4)	O(3)#2-Mn(1)-O(7)	93.8(4)
O(7)-Mn(1)-O(2)#2	89.8(4)	O(7)-Mn(1)-O(6)	177.7(4)
O(5)-Mn(1)-O(2)#2	155.1(4)	O(4)#1-Mn(1)-O(2)#2	86.7(4)
O(3)#2-Mn(1)-O(6)	88.3(4)	O(5)-Mn(1)-O(6)	92.4(4)
O(6)-Mn(1)-O(2)#2	90.3(4)	O(4)#1-Mn(1)-O(6)	90.8(4)
3			
Zn(1)-O(2)#1	1.968(5)	Zn(1)-O(4)	1.973(4)
Zn(1)-O(3)#2	2.005(5)	Zn(1)-O(7)	2.102(6)
Zn(1)-O(6)	2.224(6)	Zn(1)-O(5)#2	2.448(6)
O(2)#1-Zn(1)-O(3)#2	141.5(2)	O(2)#1-Zn(1)-O(4)	113.2(2)
O(2)#1-Zn(1)-O(7)	92.8(2)	O(4)-Zn(1)-O(3)#2	105.1(2)
O(3)#2-Zn(1)-O(7)	91.0(2)	O(4)-Zn(1)-O(7)	88.6(2)
O(4)-Zn(1)-O(6)	90.4(2)	O(2)#1-Zn(1)-O(6)	88.8(2)
O(7)-Zn(1)-O(6)	178.4(2)	O(3)#2-Zn(1)-O(6)	88.0(2)
O(4)-Zn(1)-O(5)#2	160.8(2)	O(2)#1-Zn(1)-O(5)#2	85.29(19)
O(7)-Zn(1)-O(5)#2	85.3(2)	O(6)-Zn(1)-O(5)#2	95.3(2)

对称操作码：#1 -x+1,-y+1,-z+1；#2 -x+1,-y+1,-z.

Table S2 Co^{II} geometry analysis of **1** and **1**·CH_3OH by SHAPE 2.1 software.

Compound 1		Compound 1·CH_3OH	
HP-6	32.070	32.694	
PPY-6	20.821	20.870	
OC-6	2.745	3.537	
TPR-6	10.332	8.718	
JPPY-5	24.584	25.017	

Lable	Shape	Lable	Shape	Lable	Shape	Lable	Shape	Lable	Shape
HP-6	Hexagon (D_{6h})	PPY-6	Pentagonal pyramid (C_{5V})	OC-6	Octahedron (O_h)	TPR-6	Trigonal prism (D_{3h})	JPPY-5	Johnson pentagonal pyramid (C_{5V})

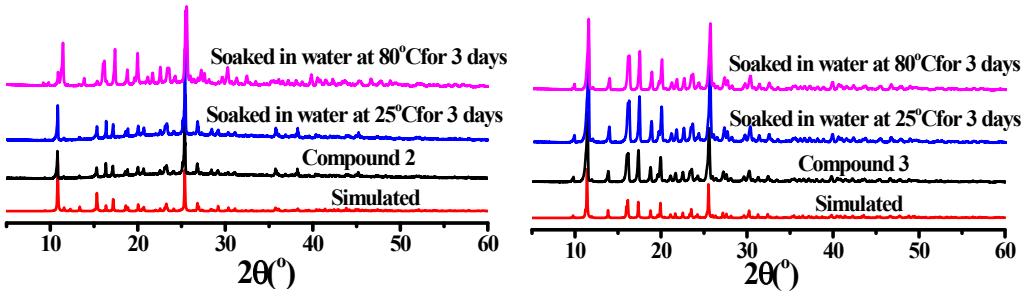

Fig. S1 Simulated (red), experimental (black), and water-treated (blue and purple) PXRD patterns of compounds **2** and **3**.

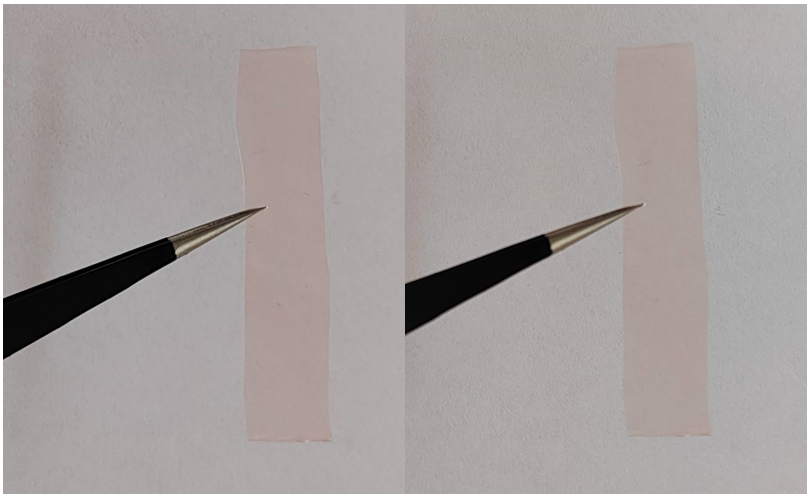

Fig. S2 The appearances of composite **1**/Nafion membranes before and after the proton conductivity studies.

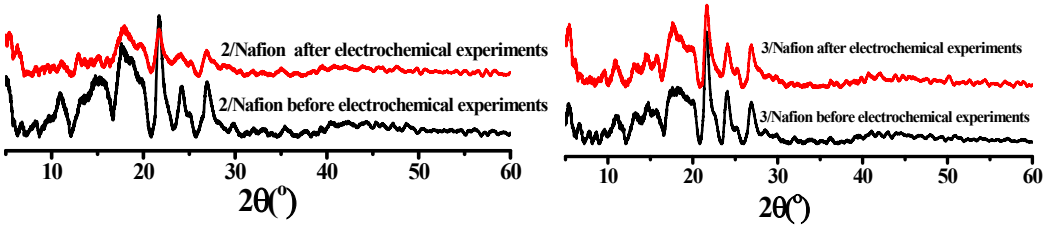

Fig. S3 The PXRD patterns of **2**/Nafion and **3**/Nafion composite membrtanes before and after electrochemical experiments.

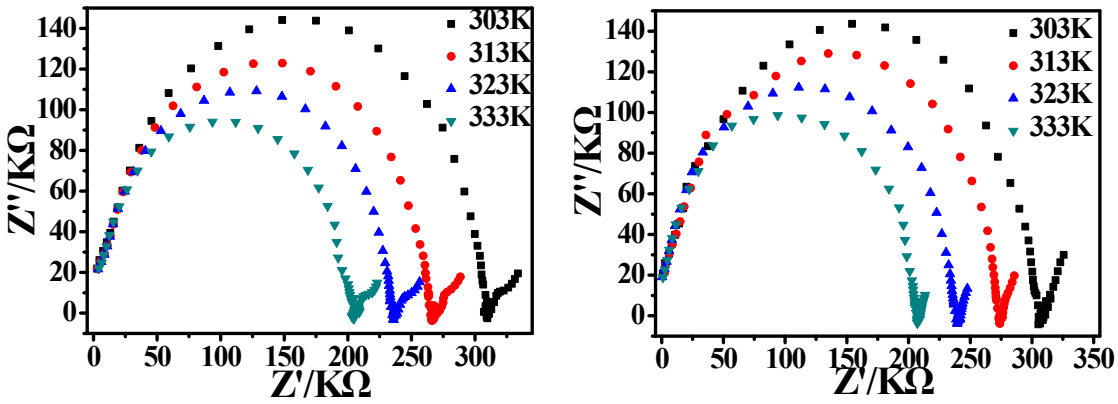

Fig. S4 The typical Nyquist plots of **2**/Nafion and **3**/Nafion at different temperature.

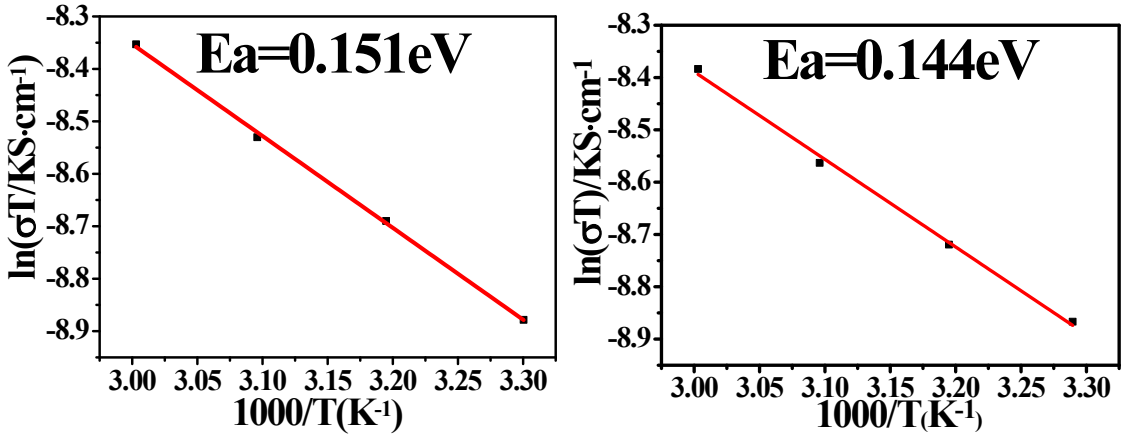

Fig. S5 The Arrhenius plots of proton conduction for **2**/Nafion and **3**/Nafion.