Supporting Information

Graphite-like polyoxometalate-based metal-organic framework as efficient anode for lithium ion batteries

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Contents

Section 1. Supplementary Structural Information

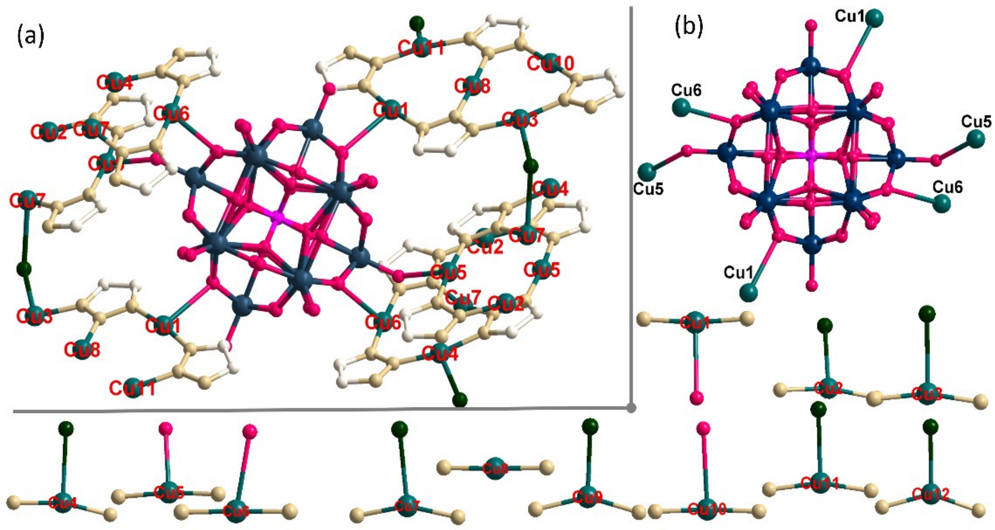

Figure S1 Ball/stick view of the crystallographic unit and the coordination patterns of PMo_{12} and Cu ions of **Cu-POM**. All of the hydrogen atoms were omitted for clarity.

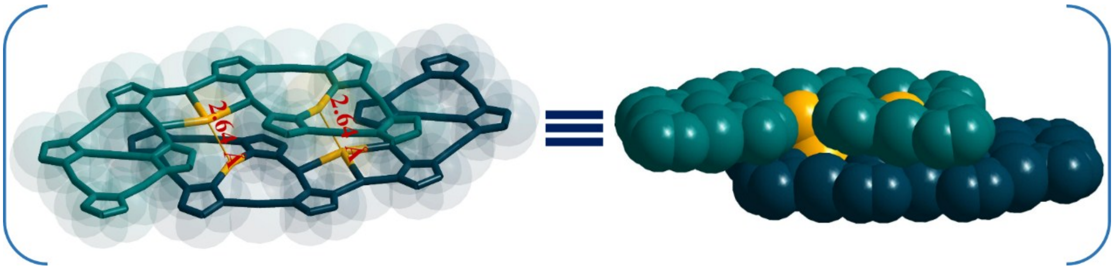

Figure S2 Combined ball/stick and stacked representation of the 1D hybrid double chains stabled by the π-π interaction between them in **Cu-POM**

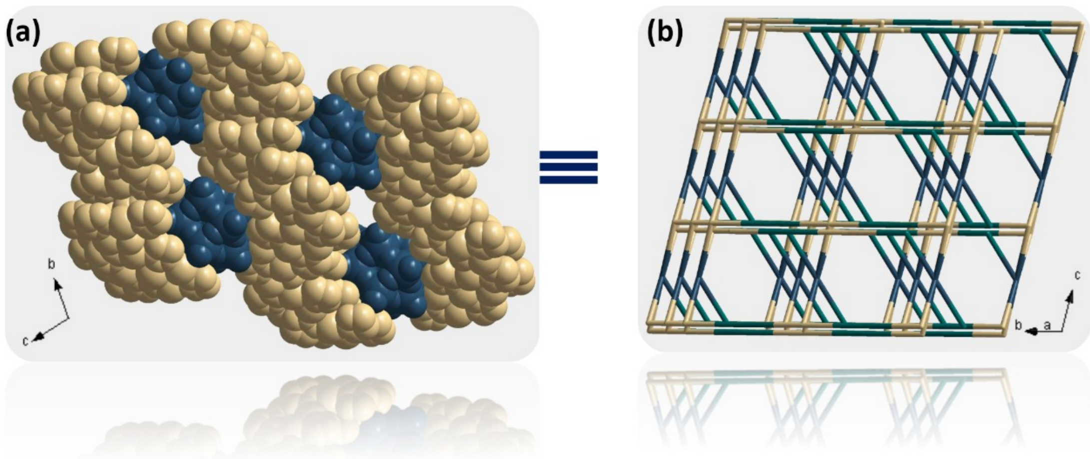

Figure S3 Combined stacked (a) and topologic (b) representation of 3D POM-based hybrid frameworks of **Cu-POM** with opening hole constructed by PMo_{12} cluster as pillars and the double chains.

Section 2 Supplementary Physical Characterizations

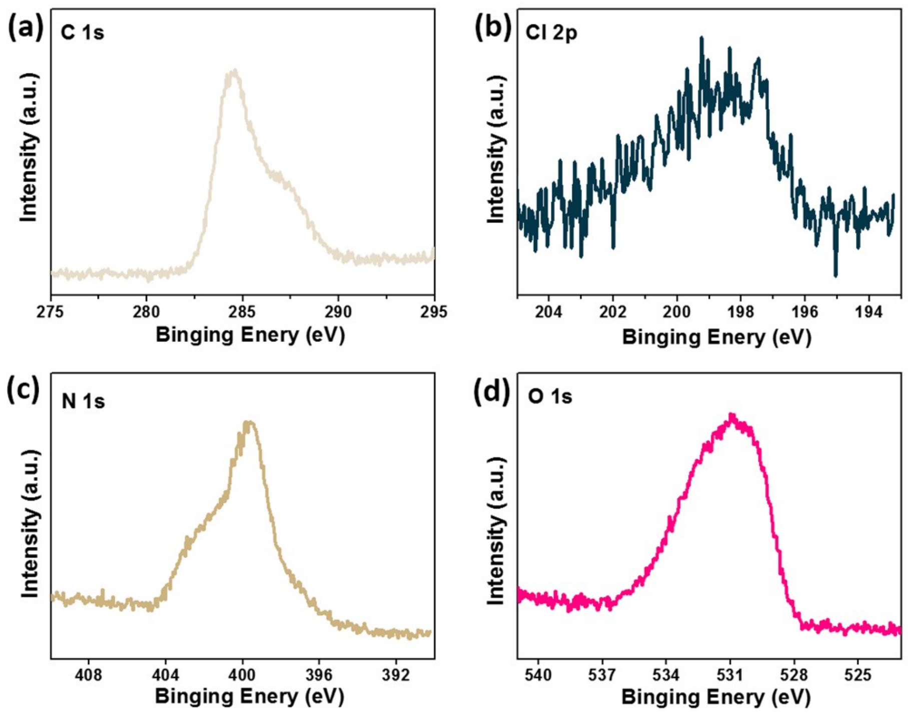

Figure S4 XPS spectra of **Cu-POM**: (a) C 1s, (b) Cl 2p, (c) N 1s, (d) O 1s, respectively.

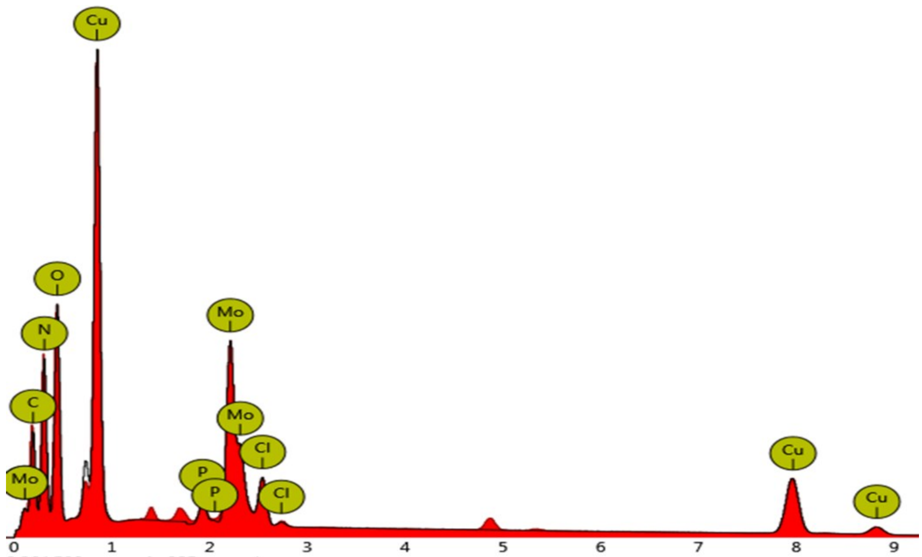

Figure S5 The EDS spectrum of **Cu-POM**.

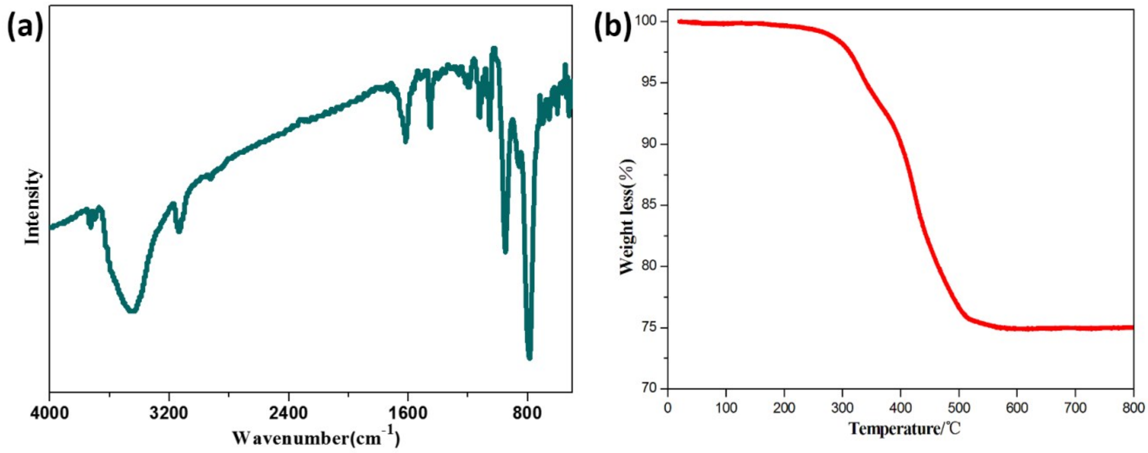

Figure S6 The FT-IR curves (a) and TG curve (b) of **Cu-POM**.

Section 3 Additional electrochemical experiments

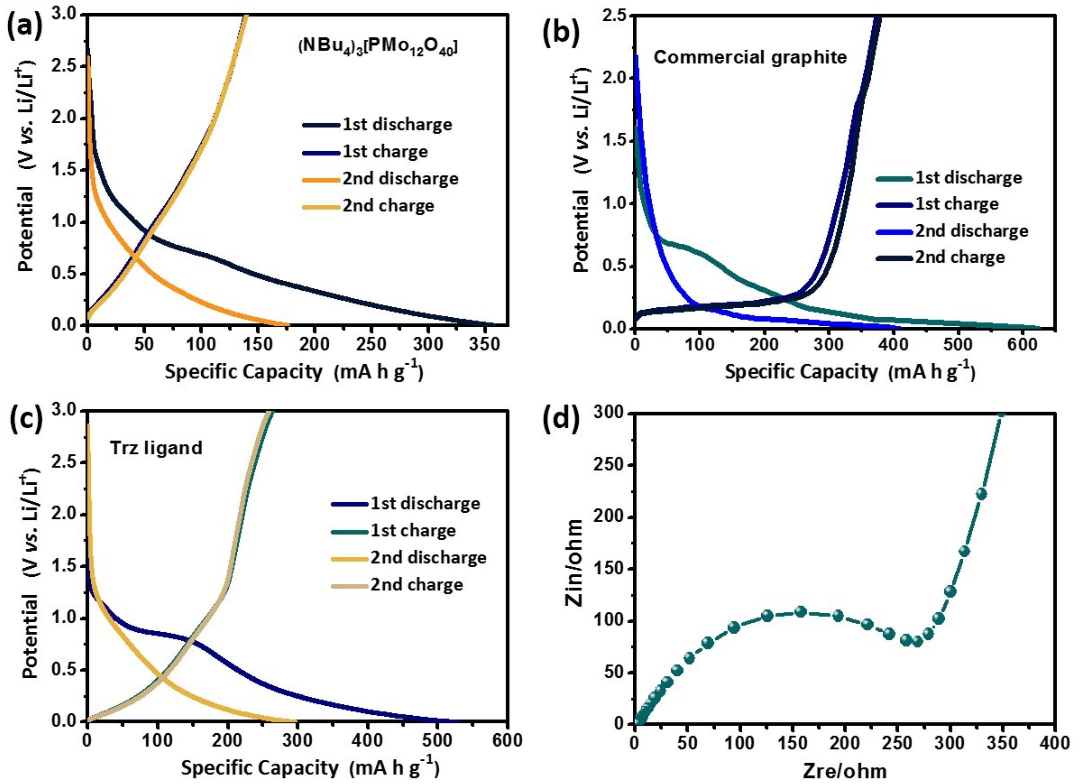

Figure S7 Charge/discharge profiles for different cycles constantly at 100 mA g^{-1} of $(NBu_4)_3[PMo_{12}O_{40}]$ (a), Trz ligand (b) and commercial graphite (c); Nyquist plots for **Cu-POM** (d) after static' 9 hours.

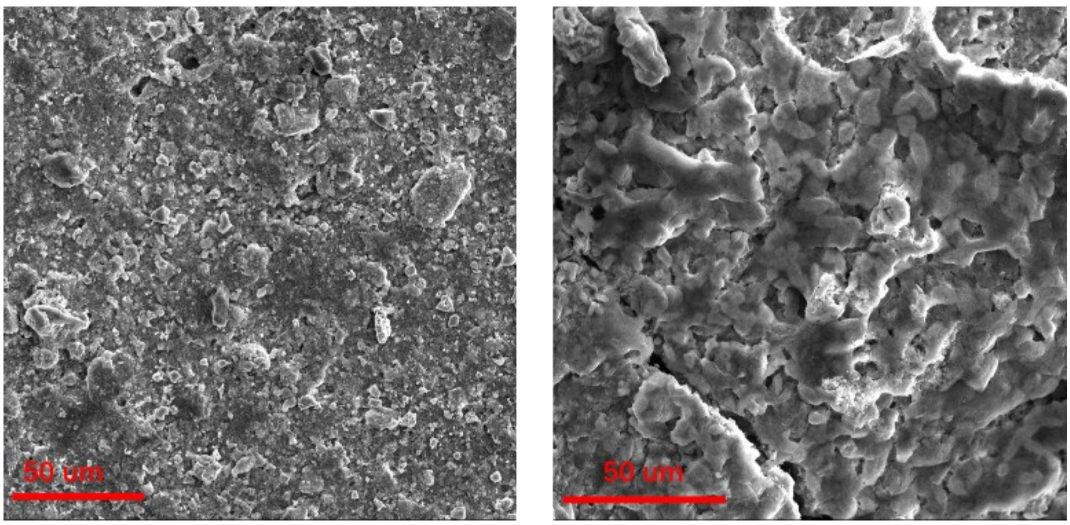

Figure S8 The SEM image of **Cu-POM**

Section 4 Bond lengths and angles for compound Cu-POM

Table S1 Bond lengths [pm] and angles [°] for **Cu-POM**

Bond	Lengths	Bond	Lengths
N(1)-N(3)	1.4(6)	N(17)-N(18)	1.57(9)
N(1)-N(2)#1	2.20(16)	N(17)-Cu(3)	2.44(9)
N(1)-Cu(7)	1.68(10)	N(18)-N(19)	1.07(9)
N(2)-N(1)#1	2.20(16)	N(18)-Cu(8)	2.01(7)
N(2)-Cu(2)	1.54(12)	N(19)-Cu(1)	1.98(8)
N(3)-Cu(6)	2.07(12)	N(20)-N(21)	1.3(2)
N(4)-N(6)#2	1.1(4)	N(20)-Cu(10)	1.86(13)
N(4)-N(5)	1.6(2)	N(21)-Cu(8)	1.72(11)
N(4)-Cu(4)	2.1(7)	N(50)-N(52)	1.29(16)
N(5)-Cu(12)	1.96(10)	N(50)-Cu(1)	1.64(14)
N(6)-N(4)#2	1.1(4)	N(51)-N(52)	1.42(10)
N(6)-Cu(6)	1.81(5)	N(51)-Cu(12)	1.78(7)
N(7)-N(8)	1.57(9)	N(52)-Cu(11)	1.96(7)
N(7)-Cu(4)#2	1.86(6)	O(1)-O(2)#3	2.06(16)
N(8)-N(9)	1.30(10)	O(1)-O(01)	1.7(2)
N(8)-Cu(7)	2.00(10)	O(2)-O(1)#3	2.06(16)
N(9)-Cu(5)	1.79(5)	O(2)-O(01)	1.49(17)
N(10)-N(21)	1.37(18)	O(20)-Cu(5)	2.40(10)
N(10)-Cu(11)	1.84(12)	Cu(2)-Cl(1)	2.630(18)
N(11)-N(13)	1.12(9)	Cu(3)-Cl(1)	2.750(17)
N(11)-N(12)	1.56(8)	Cu(4)-N(7)#2	1.86(6)
N(11)-Cu(2)	1.91(6)	Cu(4)-Cl(2)	2.74(2)
N(12)-Cu(5)#1	1.74(7)	Cu(5)-N(12)#1	1.74(7)
N(13)-Cu(9)	1.96(7)	Cu(7)-Cl(1)	2.62(2)
N(14)-N(16)	1.97(15)	Cu(9)-Cl(1)	2.41(2)
N(14)-Cu(9)	1.63(18)	Cu(9)-Cu(11)#4	2.958(15)
N(15)-N(16)	1.30(9)	Cu(11)-Cl(2)	2.64(2)
N(15)-Cu(10)	2.02(9)	Cu(11)-Cu(9)#4	2.958(15)
N(16)-Cu(3)	2.00(9)	Cu(12)-Cl(2)	2.50(2)
Bond	**Angles**	**Bond**	**Angles**
N(3)-N(1)-N(2)#1	89(9)	N(18)-N(19)-Cu(1)	118(5)
N(3)-N(1)-Cu(7)	144(10)	N(21)-N(20)-Cu(10)	124(10)
N(2)#1-N(1)-Cu(7)	112(6)	N(20)-N(21)-N(10)	109(10)
N(1)#1-N(2)-Cu(2)	115(4)	N(20)-N(21)-Cu(8)	118(10)
N(1)-N(3)-Cu(6)	93(10)	N(10)-N(21)-Cu(8)	132(9)
N(6)#2-N(4)-N(5)	112(10)	N(52)-N(50)-Cu(1)	124(6)
N(6)#2-N(4)-Cu(4)	126(10)	N(52)-N(51)-Cu(12)	159(10)

N(5)-N(4)-Cu(4)	107(10)	N(51)-N(52)-N(50)	131(9)
N(4)-N(5)-Cu(12)	123(10)	N(51)-N(52)-Cu(11)	92(7)
N(4)#2-N(6)-Cu(6)	127(10)	N(50)-N(52)-Cu(11)	136(7)
N(8)-N(7)-Cu(4)#2	118(4)	O(2)#3-O(1)-O(01)	84(8)
N(9)-N(8)-N(7)	109(6)	O(1)#3-O(2)-O(01)	92(9)
N(9)-N(8)-Cu(7)	123(8)	N(19)-Cu(1)-N(50)	165(4)
N(7)-N(8)-Cu(7)	111(6)	N(11)-Cu(2)-N(2)	168(4)
N(8)-N(9)-Cu(5)	118(5)	N(11)-Cu(2)-Cl(1)	97.0(18)
N(21)-N(10)-Cu(11)	119(8)	N(2)-Cu(2)-Cl(1)	91(2)
N(13)-N(11)-N(12)	114(6)	N(16)-Cu(3)-N(17)	147(4)
N(13)-N(11)-Cu(2)	121(5)	N(16)-Cu(3)-Cl(1)	91(2)
N(12)-N(11)-Cu(2)	121(4)	N(17)-Cu(3)-Cl(1)	97.2(15)
N(11)-N(12)-Cu(5)#1	125(5)	N(4)-Cu(4)-N(7)#2	168(4)
N(11)-N(13)-Cu(9)	133(5)	N(4)-Cu(4)-Cl(2)	104(4)
N(16)-N(14)-Cu(9)	98(8)	N(7)#2-Cu(4)-Cl(2)	87.9(17)
N(16)-N(15)-Cu(10)	136(9)	N(9)-Cu(5)-N(12)#1	171(3)
N(14)-N(16)-N(15)	116(10)	N(9)-Cu(5)-O(20)	82(4)
N(14)-N(16)-Cu(3)	133(7)	N(12)#1-Cu(5)-O(20)	99(3)
N(15)-N(16)-Cu(3)	111(8)	N(3)-Cu(6)-N(6)	165(5)
N(18)-N(17)-Cu(3)	91(5)	N(1)-Cu(7)-N(8)	149(7)
N(19)-N(18)-N(17)	99(6)	N(1)-Cu(7)-Cl(1)	100(6)
N(19)-N(18)-Cu(8)	131(5)	N(8)-Cu(7)-Cl(1)	107(4)
N(17)-N(18)-Cu(8)	108(5)	N(18)-Cu(8)-N(21)	172(5)
N(5)-Cu(12)-Cl(2)	110(2)	N(14)-Cu(9)-N(13)	132(5)
N(51)-Cu(12)-Cl(2)	93(4)	N(14)-Cu(9)-Cl(1)	129(4)
Cu(9)-Cl(1)-Cu(7)	119.5(9)	N(13)-Cu(9)-Cl(1)	97.9(16)
Cu(9)-Cl(1)-Cu(2)	87.4(6)	N(14)-Cu(9)-Cu(11)#4	88(5)
Cu(7)-Cl(1)-Cu(2)	77.3(6)	N(13)-Cu(9)-Cu(11)#4	86.1(14)
Cu(9)-Cl(1)-Cu(3)	87.1(6)	Cl(1)-Cu(9)-Cu(11)#4	110.4(7)
Cu(7)-Cl(1)-Cu(3)	116.9(7)	N(20)-Cu(10)-N(15)	165(5)
Cu(2)-Cl(1)-Cu(3)	165.6(10)	N(52)-Cu(11)-N(10)	153(3)
Cu(12)-Cl(2)-Cu(11)	82.7(6)	N(52)-Cu(11)-Cl(2)	110(2)
Cu(12)-Cl(2)-Cu(4)	82.0(6)	N(10)-Cu(11)-Cl(2)	96(2)
Cu(11)-Cl(2)-Cu(4)	154.1(9)	N(52)-Cu(11)-Cu(9)#4	96.3(19)
O(2)-O(01)-O(1)	113(10)	N(10)-Cu(11)-Cu(9)#4	81(5)
N(5)-Cu(12)-N(51)	158(5)	Cl(2)-Cu(11)-Cu(9)#4	107.7(7)

Symmetry transformations used to generate equivalent atoms: #1 -x,-y,-z+1; #2 -x+2,-y+1,-z+1; #3 -x+1; -y,-z #4 -x+1; -y+1,-z+1.