

Supporting Information:

Syntheses, structures and properties of two 2-D layered hybrid organic-inorganic materials based on different V_4O_{12} building units

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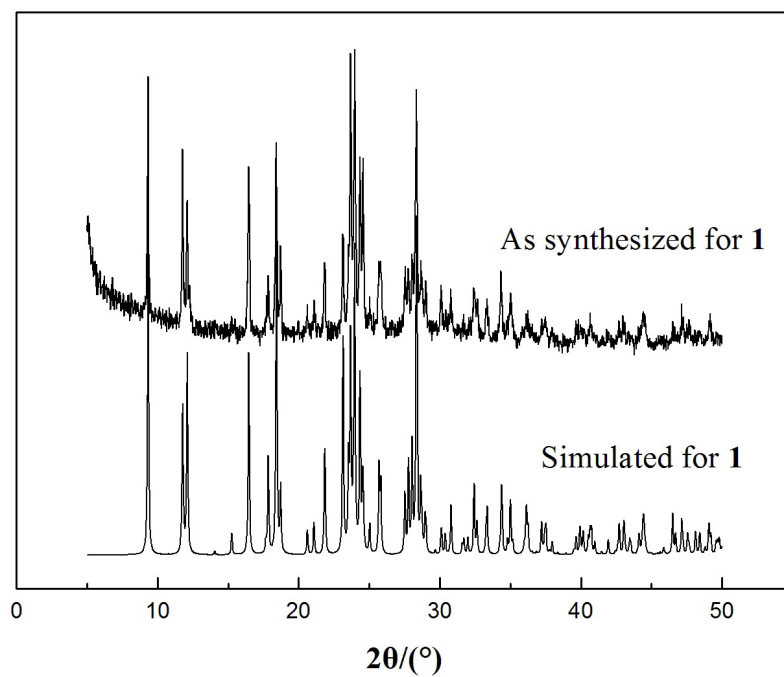


Fig. S1a PXR D patterns for compound 1.

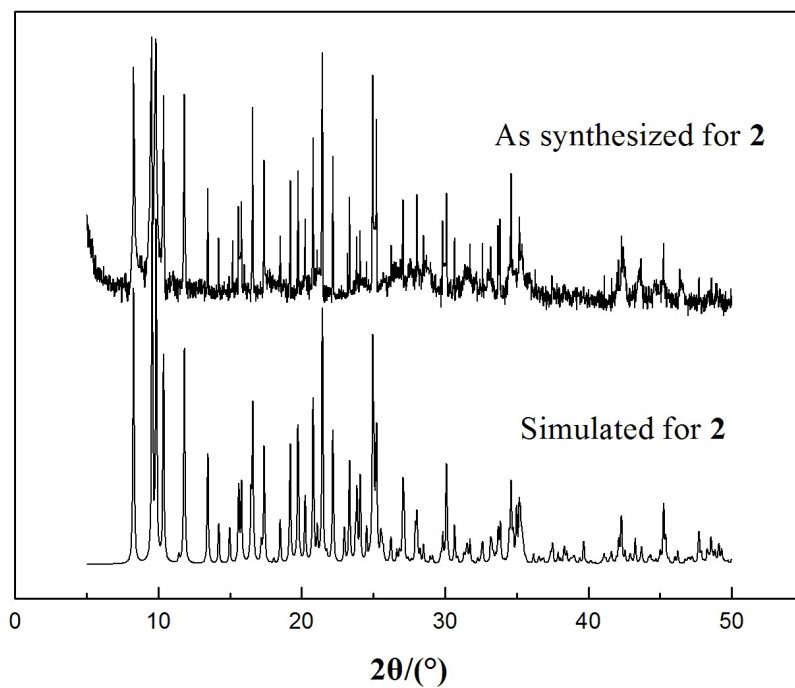


Fig. S1b PXRD patterns for compound 2.

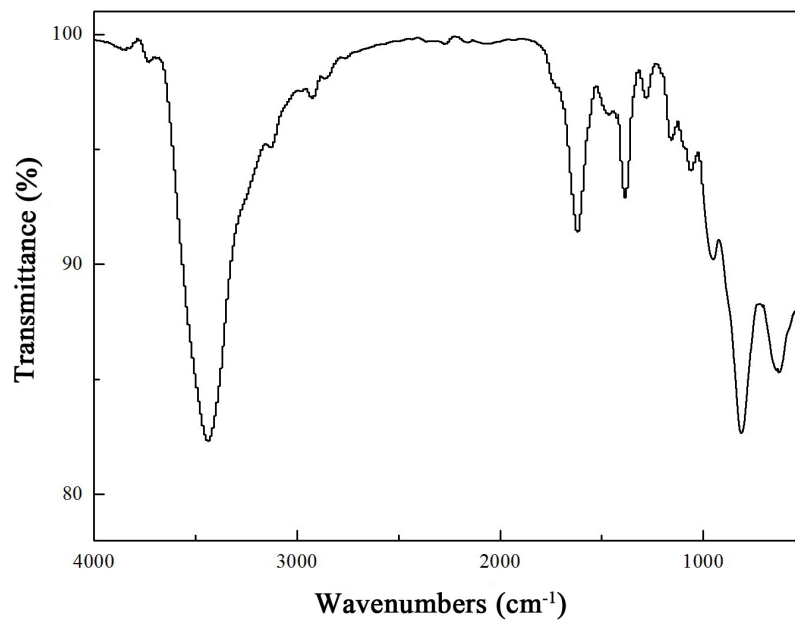


Fig. S2a The IR spectrum of compound 1.

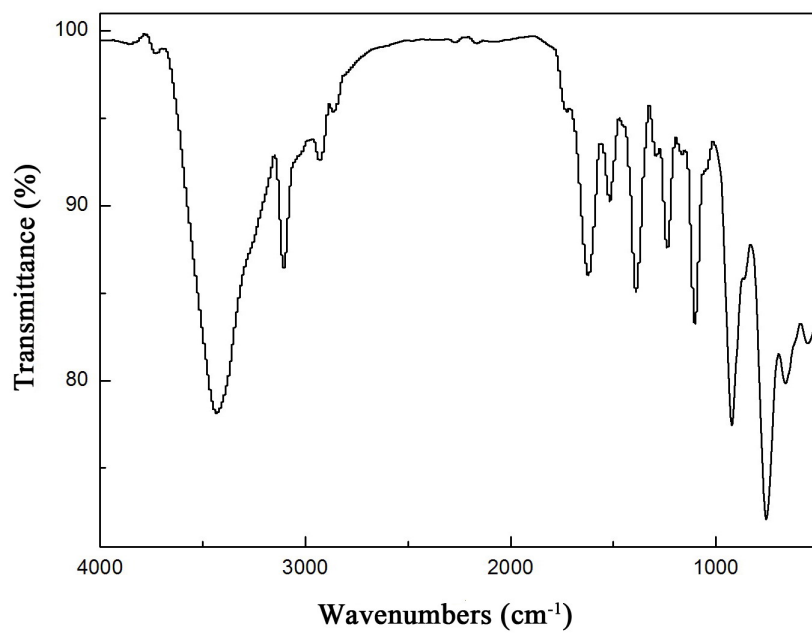


Fig. S2b The IR spectrum of compound 2.

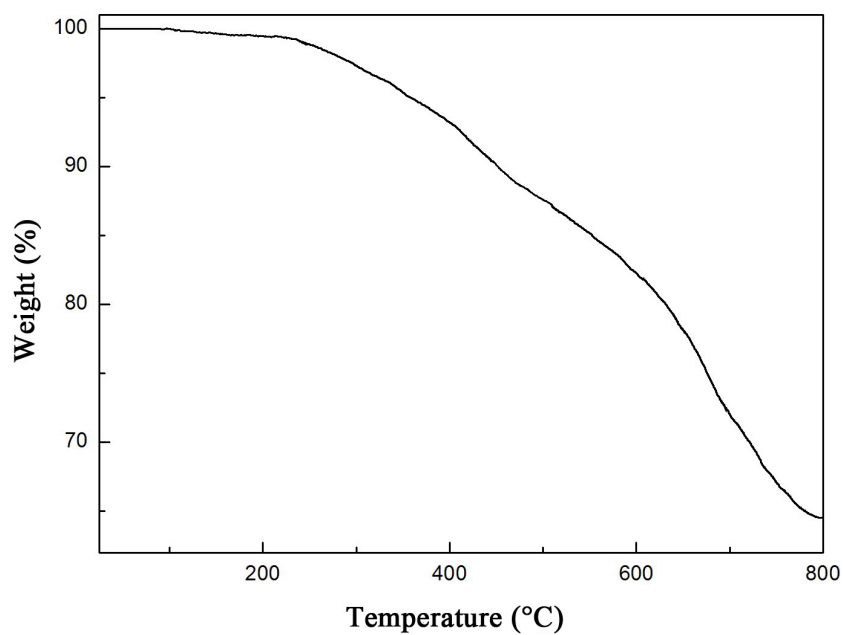


Fig. S3a TG curve for compound 1.

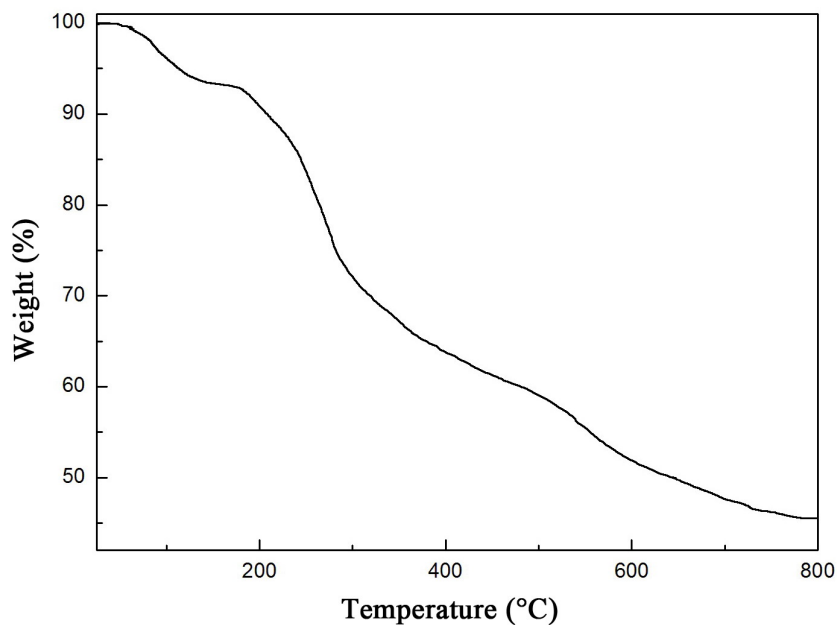


Fig. S3b TG curve for compound 2.

Table S1a Selected bond distances (Å) and angles (°) for 1

V(1)-O(7)	1.7795(10)	O(1)-V(3)#3	1.7569(11)
V(1)-O(10)	1.658(3)	O(2)-V(4)#4	1.7672(12)
V(1)-O(12)	1.640(3)	O(5)-V(3)#2	1.637(3)
V(1)-O(13)	1.780(3)	O(6)-V(4)#1	1.650(3)
V(2)-O(8)	1.7810(10)	O(7)-V(1)#5	1.7795(10)
V(2)-O(9)	1.640(2)	O(8)-V(2)#6	1.7810(10)
V(2)-O(11)	1.629(2)	Zn(1)-O(9)	2.008(3)
V(2)-O(14)	1.745(3)	Zn(1)-O(6)	2.030(3)
V(3)-O(1)	1.7569(11)	Zn(1)-O(12)	2.008(3)
V(3)-O(4)	1.622(3)	Zn(1)-N(1)	2.195(3)
V(3)-O(13)	1.801(3)	Zn(1)-N(2)	2.054(3)
V(3)-O(5)#1	1.637(3)	Zn(2)-O(5)	2.037(3)
V(4)-O(2)	1.7672(12)	Zn(2)-O(10)	1.975(3)
V(4)-O(3)	1.598(3)	Zn(2)-O(11)	2.017(3)
V(4)-O(14)	1.828(3)	Zn(2)-N(4)	2.221(3)
V(4)-O(6)#2	1.650(3)	Zn(2)-N(5)	2.044(3)
O(7)-V(1)-O(13)	108.17(9)	O(6)#2-V(4)-O(2)	108.76(13)
O(10)-V(1)-O(7)	109.44(10)	O(6)#2-V(4)-O(14)	111.56(13)
O(10)-V(1)-O(13)	110.08(14)	O(9)-Zn(1)-O(6)	98.84(13)
O(12)-V(1)-O(7)	108.78(11)	O(9)-Zn(1)-O(12)	111.22(11)
O(12)-V(1)-O(10)	109.97(15)	O(12)-Zn(1)-O(6)	93.95(12)
O(12)-V(1)-O(13)	110.36(13)	O(6)-Zn(1)-N(1)	163.18(11)
O(9)-V(2)-O(8)	109.22(9)	O(6)-Zn(1)-N(2)	91.00(11)

O(9)-V(2)-O(14)	109.11(14)	O(9)-Zn(1)-N(1)	96.50(12)
O(11)-V(2)-O(8)	109.19(11)	O(9)-Zn(1)-N(2)	108.36(11)
O(11)-V(2)-O(9)	110.79(14)	O(12)-Zn(1)-N(1)	86.87(12)
O(11)-V(2)-O(14)	110.96(13)	O(12)-Zn(1)-N(2)	138.77(12)
O(14)-V(2)-O(8)	107.49(11)	N(2)-Zn(1)-N(1)	77.60(11)
O(1)-V(3)-O(13)	107.32(9)	O(10)-Zn(2)-O(5)	101.03(13)
O(4)-V(3)-O(1)	109.29(12)	O(10)-Zn(2)-O(11)	112.12(11)
O(4)-V(3)-O(5)#1	109.30(15)	O(11)-Zn(2)-O(5)	91.58(11)
O(4)-V(3)-O(13)	110.04(15)	O(5)-Zn(2)-N(4)	160.35(12)
O(5)#1-V(3)-O(1)	112.07(12)	O(5)-Zn(2)-N(5)	91.03(12)
O(5)#1-V(3)-O(13)	108.78(12)	O(10)-Zn(2)-N(4)	97.68(13)
O(2)-V(4)-O(14)	106.42(10)	O(10)-Zn(2)-N(5)	108.01(14)
O(3)-V(4)-O(2)	106.75(12)	O(11)-Zn(2)-N(4)	86.87(12)
O(3)-V(4)-O(6)#2	111.84(15)	O(11)-Zn(2)-N(5)	138.44(14)
O(3)-V(4)-O(14)	111.21(15)	N(5)-Zn(2)-N(4)	77.44(13)

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

$-x+3,-y+1,-z$; #5 $-x+2,-y+1,-z+1$; #6 $-x+2,-y+1,-z$

Table S1b Selected bond distances (Å) and angles (°) for **2**

V(1)-O(3)	1.819(2)	Cu(1)-N(8)	2.035(3)
V(1)-O(4)	1.635(3)	Cu(1)-O(5)#1	2.393(2)
V(1)-O(5)	1.641(2)	Cu(1)-N(1)#1	1.998(3)
V(1)-O(6)	1.811(2)	Cu(1)-N(8)#1	2.035(3)
V(2)-O(1)	1.639(3)	Cu(2)-O(1W)	2.503(4)
V(2)-O(2)	1.637(3)	Cu(2)-N(5)	2.028(3)
V(2)-O(6)	1.807(2)	Cu(2)-N(4)#2	2.034(3)
V(2)-O(3)#4	1.805(2)	Cu(2)-O(1W)#3	2.503(4)
Cu(1)-O(5)	2.393(2)	Cu(2)-N(5)#3	2.028(3)
Cu(1)-N(1)	1.998(3)	Cu(2)-N(4)#1	2.034(3)
O(3)-V(1)-O(4)	110.75(14)	O(5)#1-Cu(1)-N(8)	91.61(9)
O(3)-V(1)-O(5)	107.36(12)	N(1)#1-Cu(1)-N(8)	86.66(11)
O(3)-V(1)-O(6)	111.06(11)	N(8)-Cu(1)-N(8)#1	180.00
O(4)-V(1)-O(5)	108.54(15)	O(5)#1-Cu(1)-N(1)#1	90.57(11)
O(4)-V(1)-O(6)	108.47(14)	O(5)#1-Cu(1)-N(8)#1	88.40(9)
O(5)-V(1)-O(6)	110.64(12)	N(1)#1-Cu(1)-N(8)#1	93.34(11)
O(1)-V(2)-O(2)	108.87(14)	O(1W)-Cu(2)-N(5)	90.25(11)
O(1)-V(2)-O(6)	109.44(13)	O(1W)-Cu(2)-N(4)#2	93.52(11)
O(1)-V(2)-O(3)#4	110.74(14)	O(1W)-Cu(2)-O(1W)#3	180.00
O(2)-V(2)-O(6)	108.72(12)	O(1W)-Cu(2)-N(5)#3	89.75(11)
O(2)-V(2)-O(3)#4	108.66(12)	O(1W)-Cu(2)-N(4)#1	86.48(11)
O(3)#4-V(2)-O(6)	110.37(12)	N(4)#2-Cu(2)-N(5)	87.75(12)
O(5)-Cu(1)-N(1)	90.57(11)	O(1W)#3-Cu(2)-N(5)	89.75(11)

O(5)-Cu(1)-N(8)	88.40(9)	N(5)-Cu(2)-N(5)#3	180.00
O(5)-Cu(1)-O(5)#1	180.00	N(4)#1-Cu(2)-N(5)	92.25(12)
O(5)-Cu(1)-N(1)#1	89.43(11)	O(1W)#3-Cu(2)-N(4)#2	86.48(11)
O(5)-Cu(1)-N(8)#1	91.61(9)	N(4)#2-Cu(2)-N(5)#3	92.25(12)
N(1)-Cu(1)-N(8)	93.34(11)	N(4)#2-Cu(2)-N(4)#1	180.00
O(5)#1-Cu(1)-N(1)	89.43(11)	O(1W)#3-Cu(2)-N(5)#3	90.25(11)
N(1)-Cu(1)-N(1)#1	180.00	O(1W)#3-Cu(2)-N(4)#1	93.52(11)
N(1)-Cu(1)-N(8)#1	86.66(11)	N(4)#1-Cu(2)-N(5)#3	87.75(12)

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

1-x,-1-y,-z

Table S2a Hydrogen bond interactions in compound **1**

D—H···A	H···A (Å)	D···A (Å)	D—H···A (°)
N(3)-H(3B)···O(3)	1.95	2.794(4)	167
N(6)-H(6A)···O(4)	1.97	2.812(5)	167
C(8)-H(8A)···O(9)	2.58	3.417(5)	150

Table S2b Hydrogen bond interactions in compound **2**

D—H···A	H···A (Å)	D···A (Å)	D—H···A (°)
O(1W)-H(1WA)···O(4)	1.99	2.802(5)	160
O(1W)-H(1WB)···O(7)	2.10	2.887(7)	157
C(3)-H(3A)···O(3)	2.35	3.283(4)	178
C(5)-H(5A)···O(5)	2.42	3.340(5)	170
C(7)-H(7A)···O(2)	2.29	3.186(4)	162
C(8)-H(8A)···O(4)	2.55	3.461(5)	165
C(9)-H(9A)···O(1)	2.49	3.294(6)	144
C(10)-H(10A)···O(2)	2.33	3.184(5)	153
C(11)-H(11A)···O(1)	2.58	3.522(5)	164
C(12)-H(12A)···O(2)	2.31	3.164(4)	152
C(12)-H(12A)···O(5)	2.53	3.061(4)	116
C(14)-H(14A)···O(1)	2.35	3.185(5)	150