# Electronic Supplementary Information (ESI)

# A novel 3D POMOFs based on Wells-Dawson arsenomolybdates with excellent photocatalytic and lithium-ion batteries performance

**Bo-Wen Cong,[a] Zhan-Hua Su,* [a] Zhi-Feng Zhao, *[b] and Bo Wang*[c]**

[a]*Key Laboratory of Synthesis of Functional Materials and Green Catalysis, Colleges of Heilongjiang Province, Harbin Normal University, Harbin 150025, China*

[b]*College of Material Science and Engineering, Heilongjiang University of Science and Technology, Harbin 150022, China.*

[c]*MIIT Key Laboratory of Critical Materials Technologyfor New Energy Conversion and Storage, School of Chemistry and Chemical Engineering, Harbin Institute of Technology,150001 Harbin, China.*

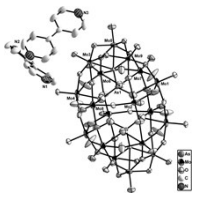
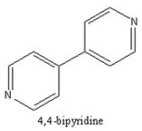
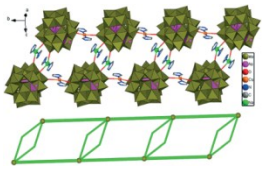
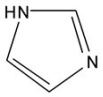
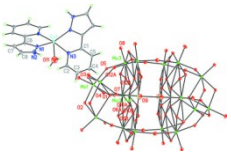
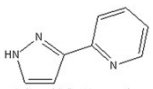
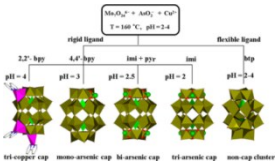
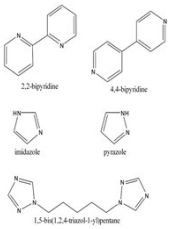
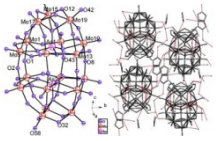
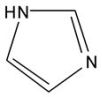
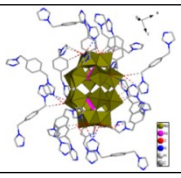
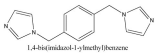
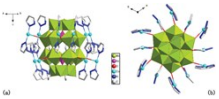
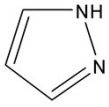
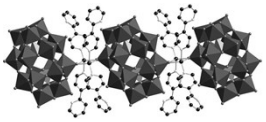
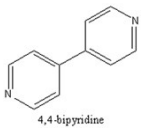
*Corresponding author. Tel: +86-0451-88060173.

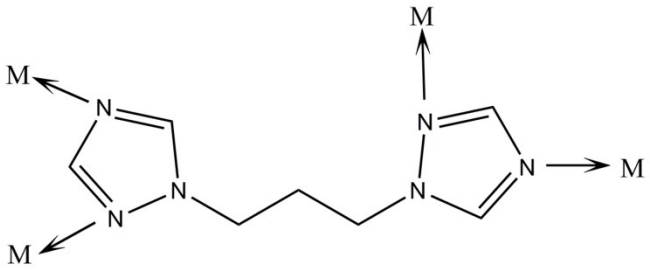
*E-mail：su_zhan_hua@163.com

*E-mail：zhifengzhao1980@163.com

*E-mail：wangbo19880804@163.com

**Table S1** The summary of organic ligands in Wells-Dawson-AMs.

| *Ref.* | *Compounds* | *Ligands* | *Ref.* | *Compounds* | *Ligands* |
|---|---|---|---|---|---|
| *27* |  |  4,4-bipyridine | *30* |  |  imidazole |
| *28* |  |  3-(2-pyridyl)-1H-pyrazole | *31* |  |  |
| *29* |  |  imidazole | *32* |  |  |
| *15* |  |  pyrazole | *33* |  |  4,4-bipyridine |




1,3-bis(1,2,4-triazol-1-yl)propane

**Fig. S1** View of the typical coordination modes of btp ligand.

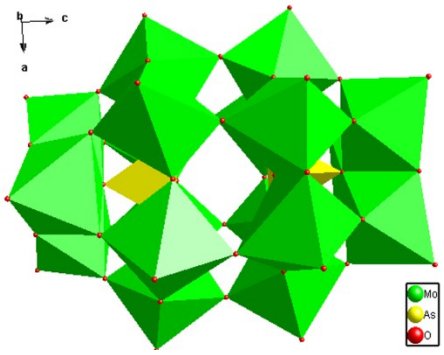



**Fig. S2** Representation of $[As_2Mo_{18}O_{62}]^{6-}$ cluster coordination polyhedron.

**Table S2.** The BVS calculation result of As Mo and Cu atoms in compound **1.**

| Code | Bond Valence |
|---|---|
| Mo1 | 6.103 |
| Mo2 | 6.267 |
| Mo3 | 5.827 |
| As1 | 5.174 |
| Cu1 | 2.057 |

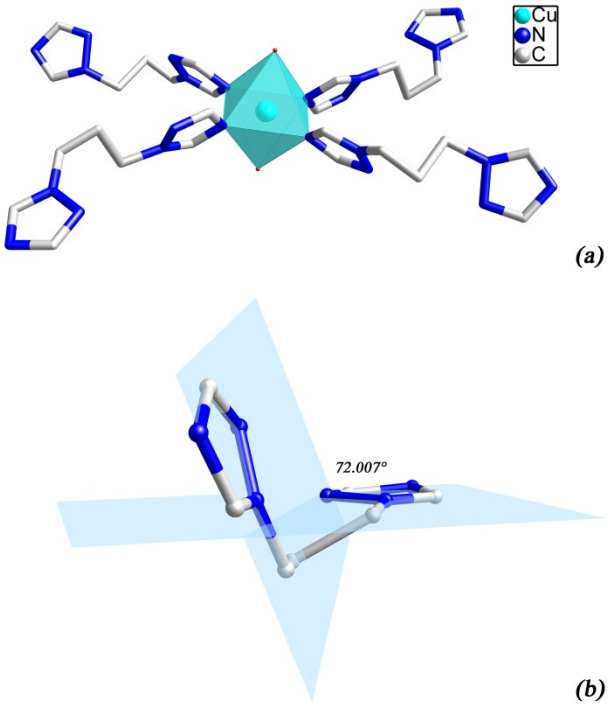



**Fig. S3** (a)The connection between copper and organic ligand btp; (b) The dihedral angles between the two triazole rings.

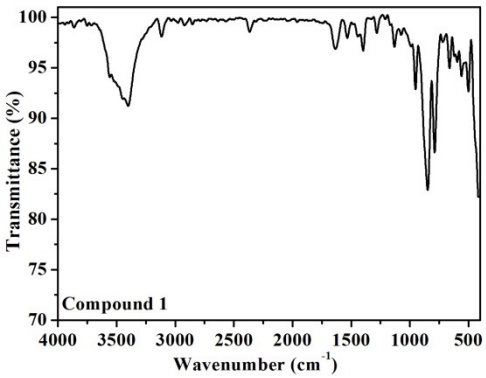



**Fig. S4** IR spectrum of compound **1**.

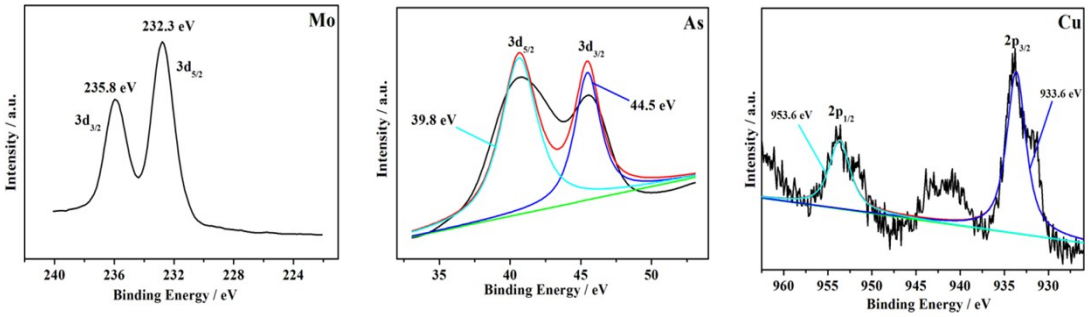



**Fig. S5** The XPS spectra of compound **1**.

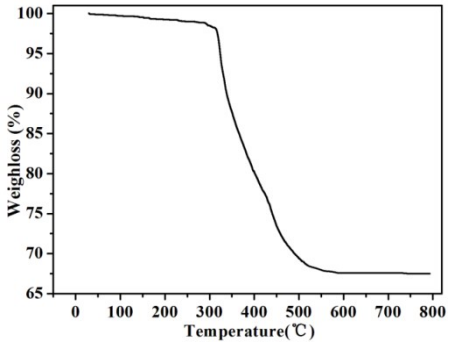



**Fig. S6** The TG curve of compound **1**.

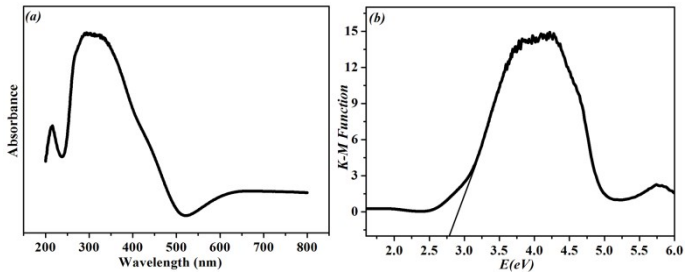



**Fig. S7** (a) The UV-vis spectra of compound **1** in solid state at room temperature; (b) *Kubelka-Munk* transformed diffuse reflectance spectrum of compound **1**.

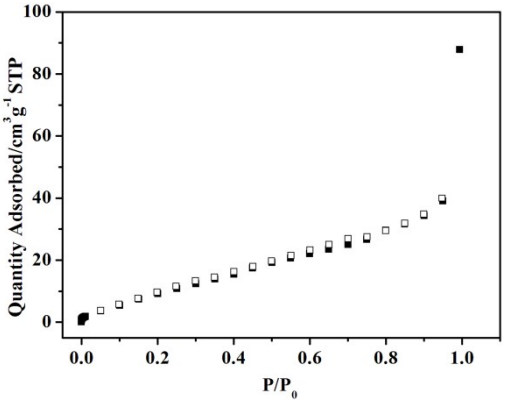



**Fig. S8** $N_2$ sorption isotherm of compound **1** at 77 K ($P_0$ = 1 atm).

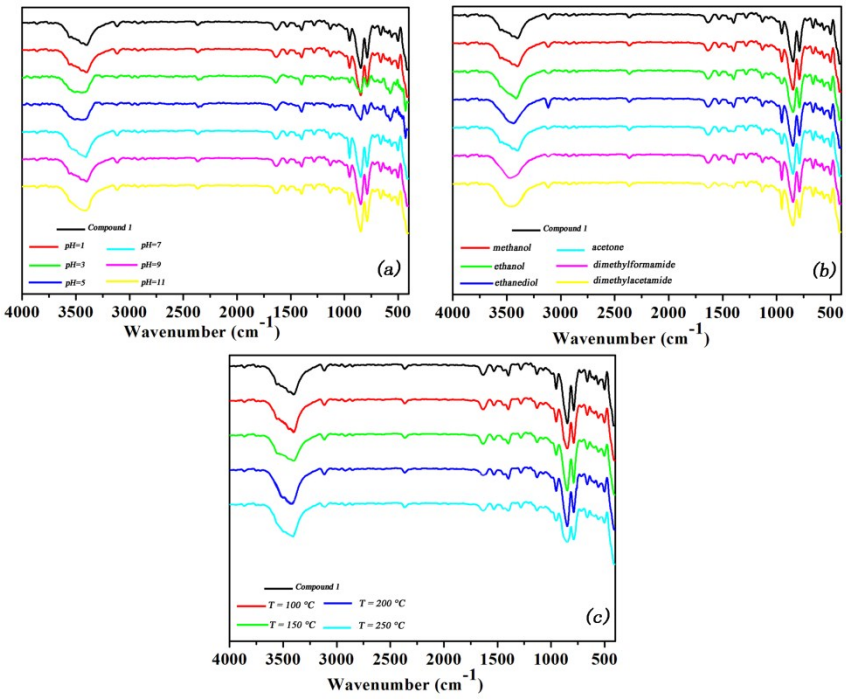



**Fig. S9** The IR spectra of compound **1** (a) immersed in aqueous solutions with different pH for 24 h; (b) soaking in different solvents for 24 h at room temperature; and (c) after heating at different temperature for 12 h, respectively.

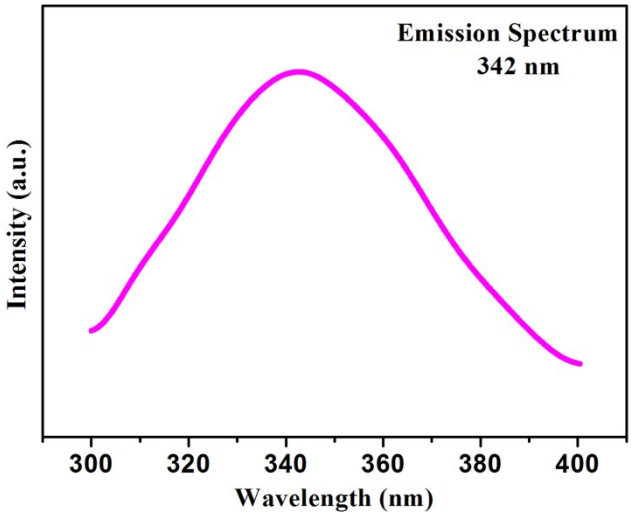



**Fig. S10** Fluorescent spectrum of compound **1**.

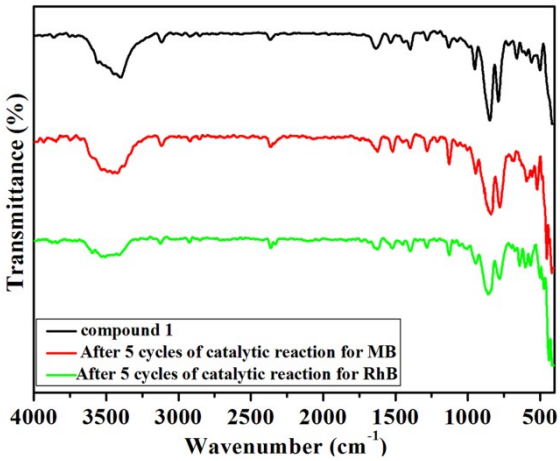



**Fig. S11** The IR spectra of compound **1** before and after cycle reaction.

**Table. S3** The fitting values of the resistance components in the simplified equivalent circuit. (In set of Fig. 7e)

| Electrode | $R_Q$/Ω·cm$^{-2}$ | $R_1$/Ω·cm$^{-2}$ | $R_2$/Ω·cm$^{-2}$ | $R_{total}$[a)]/Ω·cm$^{-2}$ |
|---|---|---|---|---|
| Before | 1.95 | 340 | 64.9 | 406.9 |
| After | 0.21 | 72.9 | 13.6 | 86.7 |

[a)] $R_{total} = R_\Omega + R_1 + R_2$.

**Table S4** Selected bond lengths (Å) and bond angles (°) of compound **1**

| | | | | | |
|---|---|---|---|---|---|
| Mo(1)-O(1) | 1.680(3) | Mo(1)-O(3) | 1.794(5) | Mo(1)-O(2) | 1.821(7) |
| Mo(1)-O(5) | 2.037(5) | Mo(1)-O(4) | 2.116(3) | Mo(1)-O(6) | 2.280(4) |
| Mo(2)-O(9) | 1.671(3) | Mo(2)-O(8) | 1.756(3) | Mo(2)-O(5) | 2.017(5) |
| Mo(2)-O(6) | 2.363(4) | Mo(3)-O(10) | 1.681(6) | Mo(3)-O(11) | 1.832(6) |
| Mo(3)-O(8) | 2.183(3) | Mo(3)-O(7) | 2.343(2) | As(1)-O(6) | 1.693(4) |
| As(1)-O(6)#3 | 1.693(4) | As(1)-O(6)#1 | 1.693(4) | As(1)-O(7) | 1.696(4) |

| | | | | | |
|---|---|---|---|---|---|
| O(1)-Cu(1) | 2.315(3) | O(2)-Mo(2)#4 | 2.089(7) | O(3)-Mo(2)#3 | 1.832(5) |
| O(4)-Mo(3)#3 | 1.824(3) | O(7)-Mo(3)#1 | 2.343(2) | O(7)-Mo(3)#3 | 2.343(2) |
| O(11)-Mo(3)#1 | 2.025(6) | Cu(1)-N(6)#5 | 2.017(12) | Cu(1)-N(1) | 2.060(5) |
| Cu(1)-N(1)#7 | 2.057(5) | N(6)-Cu(1)#8 | 2.017(12) | | |
| O(1)-Mo(1)-O(3) | 114.5(2) | O(1)-Mo(1)-O(2) | 99.6(2) | O(3)-Mo(1)-O(2) | 98.2(3) |
| O(1)-Mo(1)-O(5) | 85.7(2) | O(3)-Mo(1)-O(5) | 155.9(2) | O(2)-Mo(1)-O(5) | 90.6(3) |
| O(1)-Mo(1)-O(4) | 91.26(13) | O(3)-Mo(1)-O(4) | 87.86(18) | O(2)-Mo(1)-O(4) | 163.9(2) |
| O(5)-Mo(1)-O(4) | 78.30(17) | O(1)-Mo(1)-O(6) | 155.08(17) | O(3)-Mo(1)-O(6) | 88.2(2) |
| O(2)-Mo(1)-O(6) | 86.3(2) | O(5)-Mo(1)-O(6) | 69.96(18) | O(4)-Mo(1)-O(6) | 79.03(13) |
| O(3)#1-Mo(2)-O(5) | 149.2(2) | O(9)-Mo(2)-O(2)#2 | 90.9(2) | O(8)-Mo(2)-O(2)#2 | 163.1(2) |
| O(3)#1-Mo(2)-O(2)#2 | 64.8(2) | O(5)-Mo(2)-O(2)#2 | 97.5(2) | O(9)-Mo(2)-O(6) | 156.05(16) |
| O(8)-Mo(2)-O(6) | 87.16(14) | O(3)#1-Mo(2)-O(6) | 83.38(19) | O(5)-Mo(2)-O(6) | 68.53(18) |
| O(2)#2-Mo(2)-O(6) | 81.3(2) | O(10)-Mo(3)-O(4)#1 | 104.2(3) | O(4)#1-Mo(3)-O(11) | 95.5(3) |
| O(4)#1-Mo(3)-O(8) | 92.59(13) | O(11)-Mo(3)-O(8) | 151.0(2) | O(11)#3-Mo(3)-O(8) | 73.8(2) |
| O(10)-Mo(3)-O(7) | 170.5(3) | O(4)#1-Mo(3)-O(7) | 85.33(10) | O(11)-Mo(3)-O(7) | 74.23(19) |
| O(8)-Mo(3)-O(7) | 78.74(9) | O(6)#3-As(1)-O(6)#1 | 109.78(15) | O(6)#1-As(1)-O(6) | 109.78(15) |
| Mo(1)-O(1)-Cu(1) | 158.0(2) | Mo(1)-O(2)-Mo(2)#4 | 156.7(4) | Mo(1)-O(3)-Mo(2)#3 | 152.0(3) |
| Mo(2)-O(5)-Mo(1) | 121.7(3) | As(1)-O(6)-Mo(1) | 123.7(2) | As(1)-O(6)-Mo(2) | 118.4(2) |
| Mo(1)-O(6)-Mo(2) | 99.39(16) | As(1)-O(7)-Mo(3) | 123.59(8) | Mo(2)-O(8)-Mo(3) | 135.92(17) |
| N(6)#5-Cu(1)-N(6)#6 | 179.995(3) | N(6)#5-Cu(1)-N(1) | 95.9(11) | N(6)#6-Cu(1)-N(1) | 84.1(11) |
| N(1)-Cu(1)-N(1)#7 | 179.997(3) | | | | |

Symmetry transformations used to generate equivalent atoms: #1 -y+1,x-y,z; #2 x-y+1/3,x-1/3,-z+5/3; #3 -x+y+1,-x+1,z; #4 y+1/3,-x+y+2/3,-z+5/3; #5 -y+4/3,x-y+2/3,z+2/3; #6 y+1/3,-x+y+2/3,-z+2/3; #7 -x+5/3,-y+4/3,-z+4/3; #8 -x+y+2/3,-x+4/3,z-2/3