Supporting Information

Hydrophobic porphyrin MOFs and its catalytic characteristic on CL-20 by promoting decomposition.

Taihe Wang[a,b,1], Chengling Zou[a], Yu Li[a], Yuxin Mu[a,], Jiale Wei[a], Chao Chen [b], Yan Zhang[b], Haijian Li[b,], Jianhua Yi[b,*], Haixia Ma[a,c,*],Fengqi Zhao [b,*]*

T. H. Wang, C. L. Zou, Y. Li, Y. X. Mu, J. L Wei, Prof. H. X. Ma

[a] Xi'an Key Laboratory of Special Energy Materials, School of Chemical Engineering, Northwest University, Xi'an 710069, China

C. Chen, Y. Zhang, Prof. H. J. Li, Prof. J. H. Yi, Prof. H. X. Ma, F. Q. Zhao

[b] National Key laboratory of Energetic Materials, Xi'an Modern Chemistry Research Institute, Xi'an 710065, China

[c] Zhijian Laboratory, Xi'an 710025, China

*Corresponding authors:

H. Li (E-mail:h.j.li@outlook.com), H. Yi (E-mail: npecc_yjh2819@163.com);

H. Ma (E-mail: mahx@nwu.edu.cn), F. Zhao(E-mail:npecc@163.com)

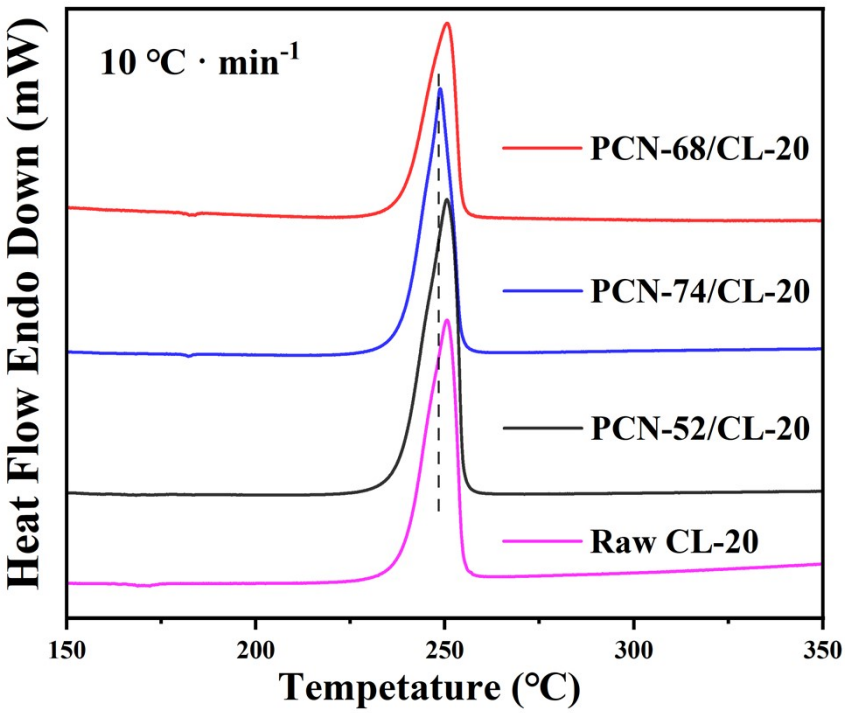

Fig. S1 DSC curves of PCN-74/CL-20, PCN-68/CL-20 PCN-54/CL-20 and raw CL-20 at the heating rate of 10 ℃·min^{-1}.

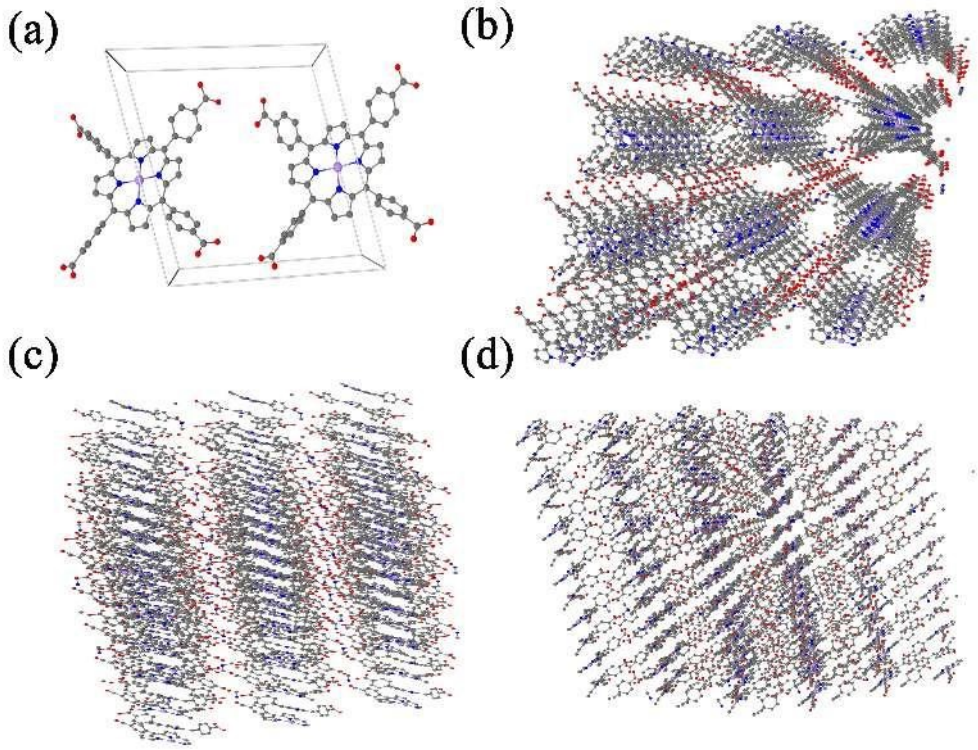

Fig. S2. (a), (b), (c), (d) The different direction view of PCN-74

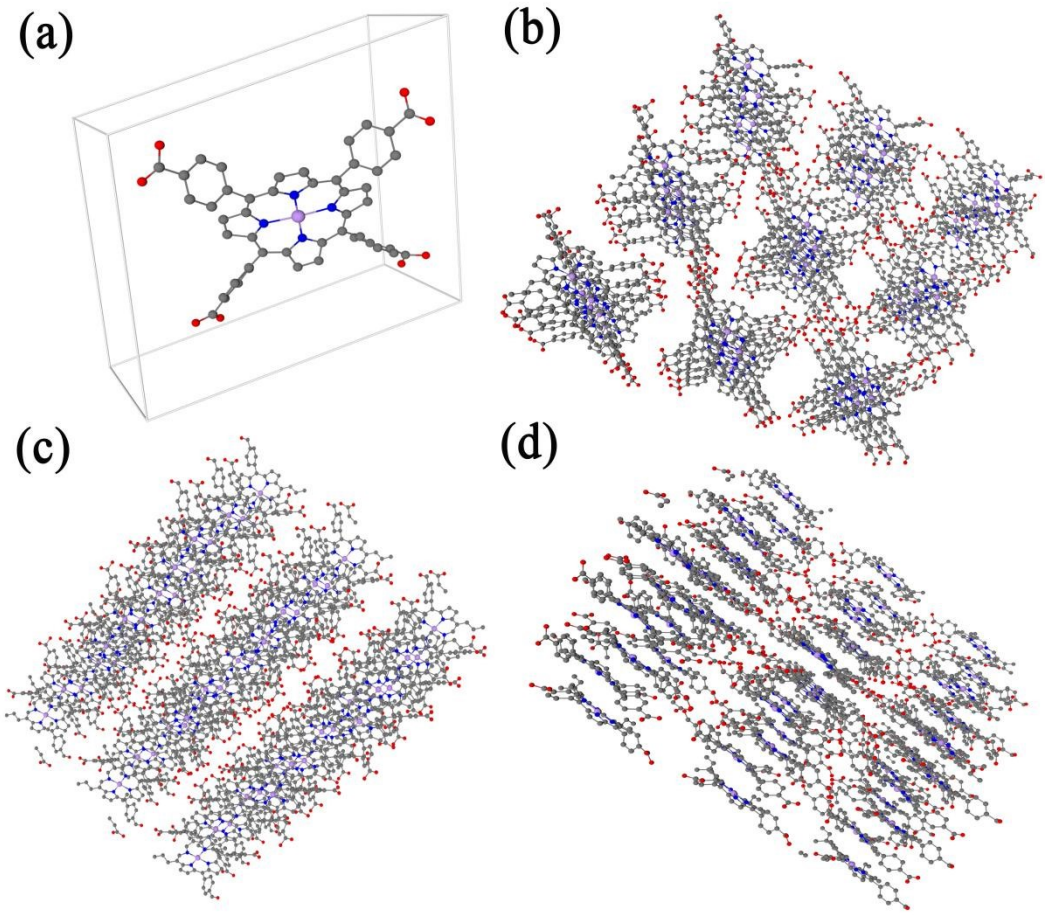

Fig. S2. (a), (b), (c), (d) The different direction view of PCN-68.

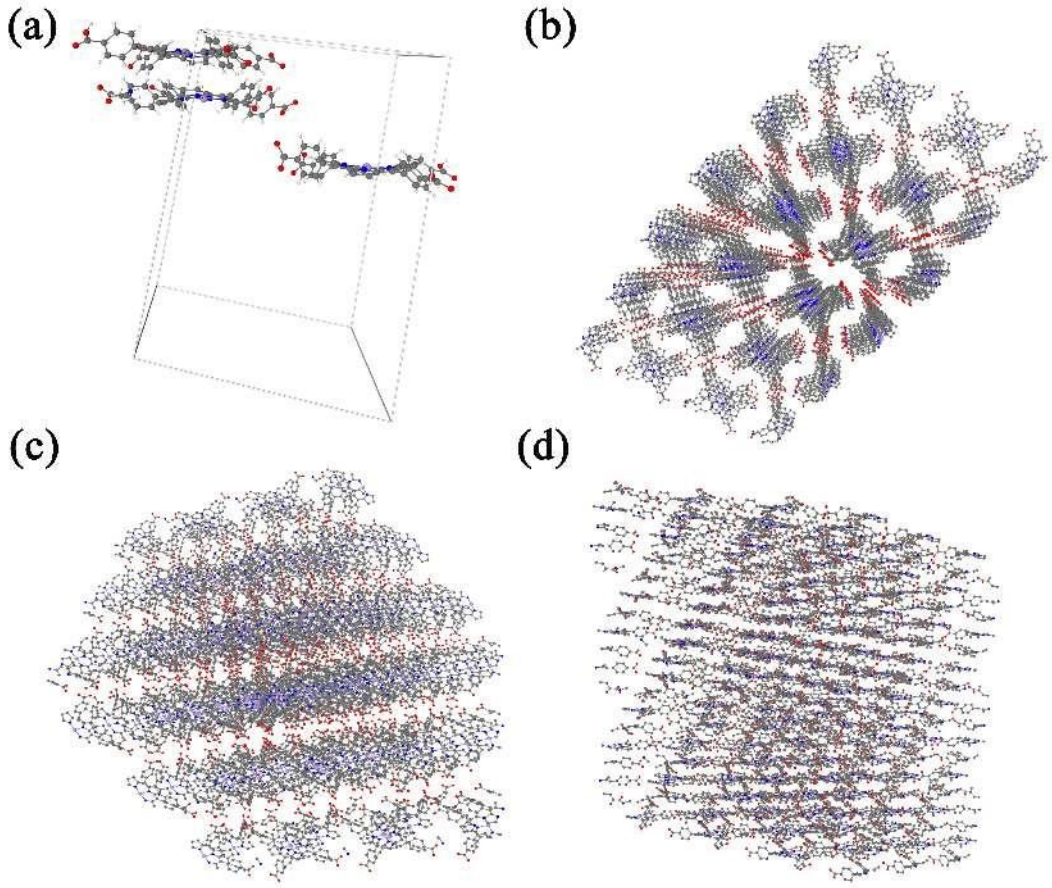

Fig. S4. (a), (b), (c), (d) The different direction view of PCN-52

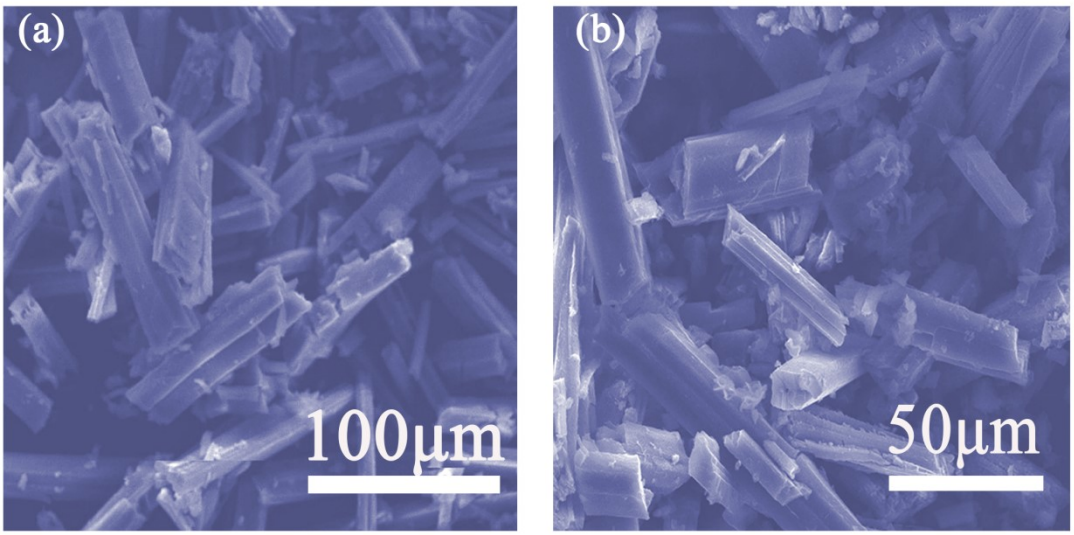

Fig. S5. Different resolution SEM images of (a), (b) PCN-74

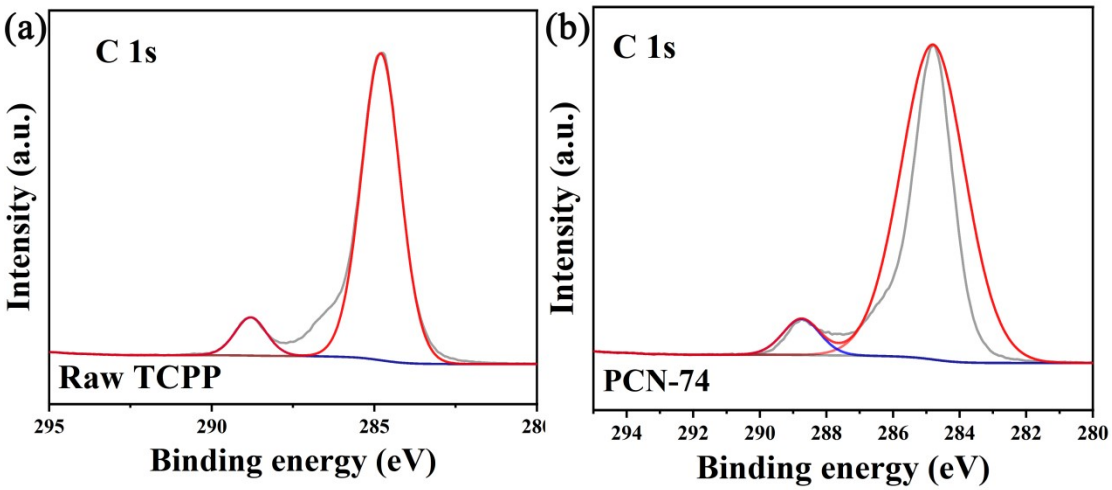

Fig. S6. High-resolution XPS survey spectra of C 1s

Table S1 Assignment of the XPS peaks for Rude TCPP and TCPP Cu MOFs

Samples	XPS peaks (eV)	Assignment	Reference
Raw TCPP	288.83	C 1s (sample C)	
	533.40, 531.86	O 1s (C-OH,C=O)	[1]
	399.70, 397.49	N 1s (C=N,C-N)	[2]
PCN-74	288.71	C 1s (sample C)	
	533.43, 531.86	O 1s (C-OH,C=O)	[3]
	399.71, 398.30	N 1s (C=N,N-Cu)	[3,4]
	932.71, 953.4 934.54, 954.42 939.6 and 943.91	Cu 2p(Cu+) Cu 2p(Cu+) Satellite	[4,5]

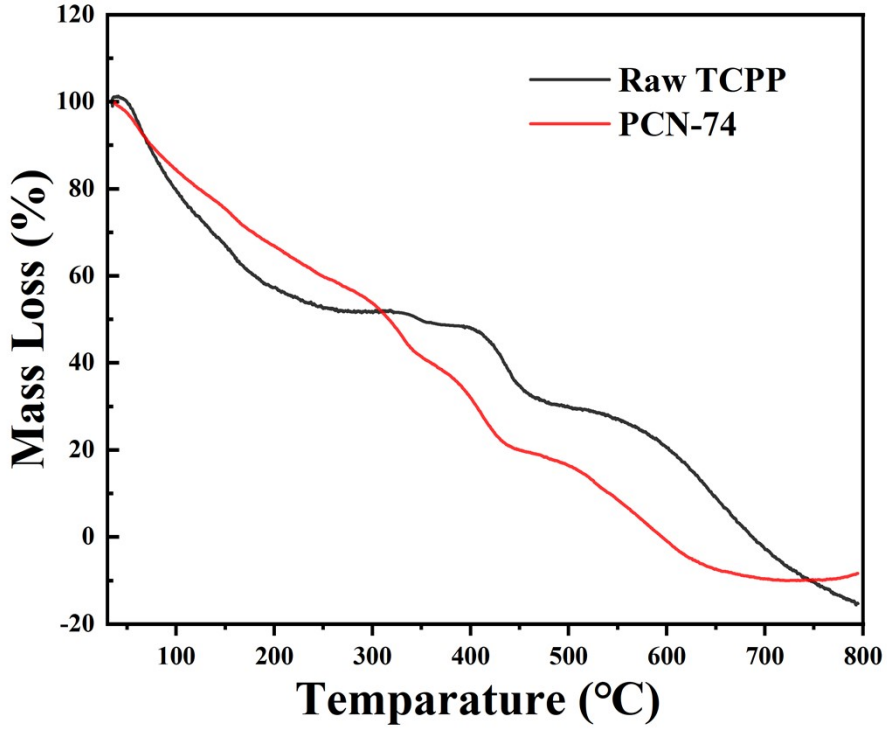

Fig. S7. TG curves of TCPP and PCN-74 at a heating rate of 10 °C·min^{-1}

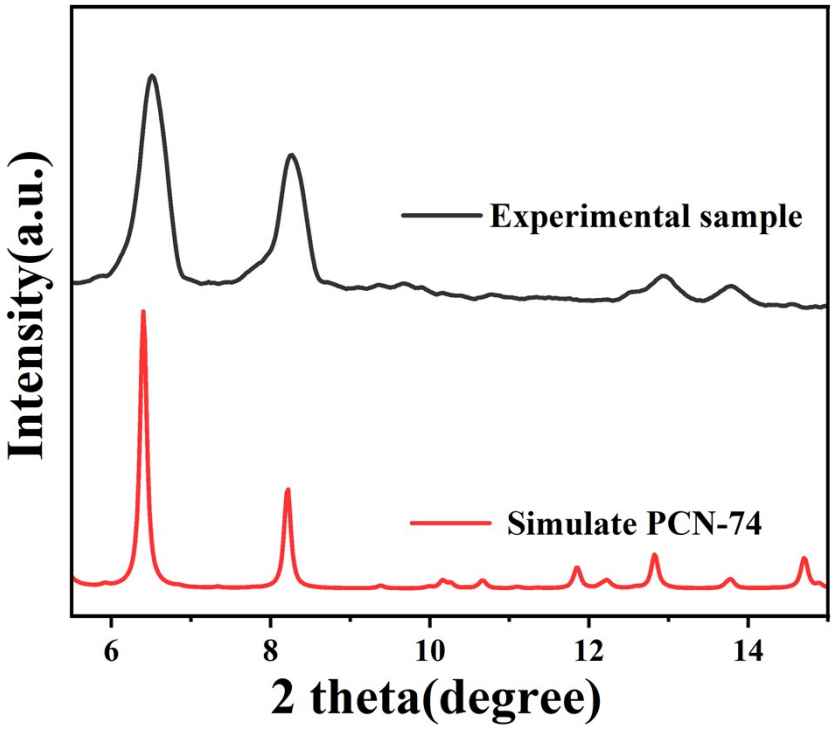

Fig.S8. The zoomed-in PXRD patterns of the PCN-74

Table. S2 Thermolysis peak temperatures and heat release.

Samples	β/℃·min^{-1}	T_0/℃	T_1/℃	ΔH/J • g^{-1}
CL-20	2.5	170.86	235.5	2783
	5	171.33	243.3	2730
	7.5	171.63	248.4	3097
	10	171.88	251.2	2429
PCN-74/CL-20	2.5	180.81	233.8	2201
	5	181.79	242.5	4052
	7.5	182.83	248.9	2277
	10	183.7	250.8	2366

Table. S3 A comparison of the molar ratio of decomposition gaseous products

	Gas production ration(%)							
	28 (N_2/CO)	16(O^+/ NH_2^+)	17 (NH_3/ OH)	18 (H_2O)	27 (HCN)	30 (CH_2O/ NO)	44 (CO_2/ N_2O)	46 (NO_2)
CL-20	34.6824	2.6581	2.8024	8.8058	22.2038	17.5666	6.3750	4.0915
PCN-74 /CL-20	25.9947	2.7207	3.3868	12.5956	19.2663	24.1913	9.4995	1.6503

In the laser ignition experiment, the PCN-74/CL-20 mixture was put in the cylindrical crucible. The sample mass is about 28-33mg. Each sample was subjected to at least four repeated parallel tests at different power densities. Due to the high sensitivity of CL-20, the mixture was only gotten some slight shaking to ensure safety. Its geometry is close to the cylindrical container.

Table. S4. The ignition delay time of CL-20 at different laser powder density.

CL-20						
Laser Power Density (W/cm^2)	**Ignition delay time 1(ms)**	**Ignition delay time 2(ms)**	**Ignition delay time 3(ms)**	**Ignition delay time 4(ms)**	**Avg(ms)**	**S.D.(ms)**
130.86634	173	176	175	170	173.5	2.64575
191.71925	98	95	97	96	96.5	1.29099
252.57217	91	92	94	90	91.5	1.70783
275	83	80	82	85	82.5	2.08167
323.56723	82	79	82	83	81.5	1.73205

Table. S5. The ignition delay time of CL-20 at different laser powder density.

PCN-74/CL-20						
Laser Power Density (W/cm^2)	**Ignition delay time 1(ms)**	**Ignition delay time 2(ms)**	**Ignition delay time 3(ms)**	**Ignition delay time 4(ms)**	**Avg(ms)**	**S.D.(ms)**
70.01343	182	185	178	188	183.25	4.272
130.86634	82	96	88	99	91.25	7.71902
191.71925	59	60	62	60	60.25	1.25831
252.57217	59	60	56	58	58.25	1.70783
275	46	49	49	48	48	1.41421

Table. S6. Comparison of activation energy has been reported for catalytic CL-20.

Sample	E/(kJ • mol^{-1})	ΔE /(kJ • mol^{-1})
This work	166.5	-13.5
5% carbon nanotubes/CL-20[6]	172.2	-12.32
Cr_2O_3/CL-20[7]	175.6	-9.6
$ZnCo_2O_4$(HCs)/CL-20[8]	148.82	-6.23
MnO_2/CL-20[9]	179.18	-8.42
6%MOF-199/CL-20[10]	161.8	-8.8
PbBa-MOF/CL-20[11]	230.99	-23.76
NiBa-MOF/CL-20[11]	212.74	-42.01
ZIF-67/CL-20[12]	179.08	-25.92
$K_2Ba[Ni(NO_2)_6]$/ CL-20[13]	277.85	+88.32
$Cu(1\text{-}MIM)_2(N_3)_2$/CL-20[14]	186.1	-9
$[Cu(1\text{-}VIM)_2(N_3)_2]n$/CL-20[14]	171.2	-23.9
nmT-Fe_2O_3/CL-20[15]	177.84	-3.35
nmG-Fe_2O_3/CL-20[15]	176.11	-5.08
nano-$CuCr_2O_4$/CL-20[16]	230.3	-25.2
nano-$NiCr_2O_4$/CL-20[16]	232.8	-23.7
nano-$ZnCr_2O_4$/CL-20[16]	252.8	-2.7

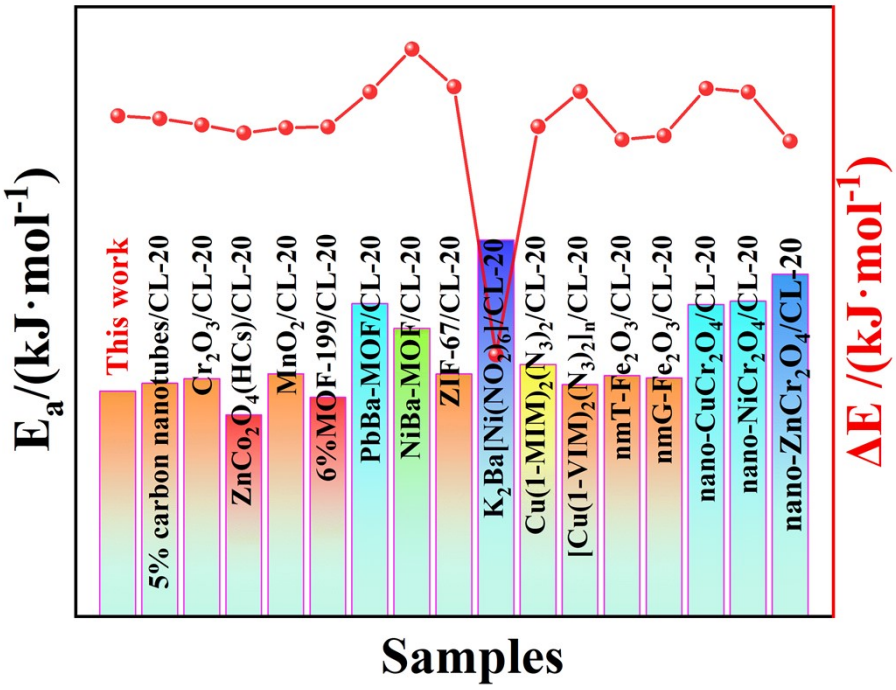

Fig. S9. Comparison of activation energy has been reported for catalytic CL-2

Reference

1 M. Xu, X. Liu, Z. Zhao, L. Sun, L. Liu, J. Guo and J. Sha, *Chem. Eng. J.*, 2024, **491**, 152178.

2 J. Wang, Z. Song, M. He, Y. Qian, D. Wang, Z. Cui, Y. Feng, S. Li, B. Huang, X. Kong, J. Han and L. Wang, *Nat. Commun.*, 2024, **15**, 2125.

3 W. Bai, S. Li, J. Ma, W. Cao and J. Zheng, *J. Mater. Chem. A*, 2019, **7**, 9086–9098.

4 Y. Liu, Y. Wei, M. Liu, Y. Bai, X. Wang, S. Shang, C. Du, W. Gao, J. Chen and Y. Liu, *Adv. Mater.*, 2021, **33**, 2007741.

5 D. D. La, H. P. N. Thi, Y. S. Kim, A. Rananaware and S. V. Bhosale, *Appl. Surf. Sci.*, 2017, **424**, 145–150.

6 X. Yu, *Chin. J. Explos. &Propellants*, 2004, **27**, 78–80.

7 N. Zhao, H. Ma, E. Yao, T. An and F. Zhao, *Chin. J. Explos. &Propellants*, 2026, **49**, 45–54.

8 Y. Li, T. Zhang, C. Li, W. Wang, A. Pang, Z. Guo and H. Ma, *Chin. J. Energ. Mater.*

9 J. Liu, N. Zhao, F. Zhao, J. Song and H. Ma, *Chin. J. Explos. Propellants*, DOI:10.14077/j.issn.1007-7812.2015.02.004.

10 H. Li, W. Tong, Z. Yan, L. Li, S. Wang, J. Huo, L. Yang, J. Han, X. Ren and W. Li, *ACS Appl. Mater. Interfaces*, 2023, **15**, 41850–41860.

11 C. Chen, H. Li, J. Yi, Z. Qin, C. Wang, Z. Sun, Y. Xu, S. Xu and F. Zhao, *Mater. Today Chem.*, 2022, **23**, 100676.

12 X. Yang, B. Tan, B. Wang, L. Yao, X. Li, D. Zhao, W. Li, L. Cao, Y. Huang and X. Wang, *Molecules*, DOI:10.3390/molecules27238370.

13 C. Chen, H. Li, Z. Qin, C. Wang, Y. Xu, Z. Sun, S. Xu, J. Yi and F. Zhao, *J. Phys. Chem. Solids*, 2022, **161**, 110411.

14 H. Li, W. Zhang, Z. Wei, L. Xia, M. Long, Z. Li and T. Zhang, *Eur. J. Inorg. Chem.*, 2022, **2022**, e202200008.

15 R. Gao, N. Zhao, J. Liu, T. Zhang and H. Ma, *Propellants Explos. Pyrotech.*, 2016, **41**, 936–941.

16 Y. Wang, T. An, N. Yan, Z. Yan, B. Zhao and F. Zhao, *ACS Omega*, 2020, **5**, 327–333.