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Electronic Supplementary Information

Photoinduced synergistic catalysis on Zn single-atom-loaded hierarchical porous carbon for highly efficient CO_2 cycloaddition conversion

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Part Ⅰ. Experimental section

Chemicals and Materials. All reagents were purchased from Sigma-Aldrich Shanghai Trading Co. Ltd (Shanghai, China) without further treatment: Zinc sulfate Heptahydrate ($ZnSO_4·7H_2O$, 99%), 1H-1,2,3-triazole ($C_2H_3N_3$, 98%), N,N-dimethylformamide (DMF, AR), ethanol (C_2H_5OH, AR), ammonium hydroxide ($NH_3·H_2O$, 25-28%), ethyl acetate, glycidol, epichlorohydrin, 3-bromopropylene oxide, hydrochloric acid (HCl, AR), sodium hydroxide (NaOH, AR), hydrofluoric acid (HF, AR), tetrabutylammonium bromide (TBAB, AR). Deionized water (18.24 MΩ·cm) was used throughout the work.

Preparation of $Zn(C_2N_3H_2)_2$ (MET-6). The energetic MOF named MET-6 was prepared according to the reported literature.[1] Briefly, $ZnSO_4·7H_2O$ (10.5 g) was dissolved in a solvent mixture containing water (120 mL), ethanol (50 mL) and DMF (50 mL). Then, 20 mL $NH_3·H_2O$ was slowly added to the above mixture with stirring. In the process of adding $NH_3·H_2O$, the mixture would be turbid and gradually become clear again. Under continuous stirring, 6.26 mL 1H-1,2,3-triazole was added dropwise to the mixture and reacted for 24 h. After that, the white target product was repeatedly washed three times by centrifugation (3000 rpm, 10 min). Finally, the as-prepared white MET-6 powder was obtained after vacuum drying (60 ℃, 8 h).

Preparation of Zn single-atom-loaded N-doped carbon (Zn SA-NC). For the synthesis of Zn SA-NC, the prepared MET-6 was transferred into a ceramic boat and placed in a temperature-programmed tube furnace. The sample was heated to 800 ℃ for 2h to carbonize MET-6 and form Zn-N_4 sites (heating rate: 5 ℃/min, under a flowing argon atmosphere). Then, the temperature was increased to 950 ℃ for another 2 h to

further stabilize the Zn-N structure and remove the residual metal phase Zn by evaporation (heating rate: 5 ℃/min, under a flowing argon atmosphere). After naturally cooling to room temperature, Zn SA-NC was directly obtained.

Preparation of porous N-doped carbon (P-NC). A series of chemical treatments were carried out to remove Zn atoms loaded in Zn SA-NC. Briefly, 100 mg Zn SA-NC was immersed in 20 mL HCl (1 M) aqueous solution with stirring at 80 ℃ for 5 h. After centrifugation and washing with water for three times, the above operation was repeated once except that 1 M HCl was replaced by 1 M NaOH. Finally, the sample was etched in a solution containing 8 mL H_2O and 2 mL HF at 80 ℃ for another 5 h. After washing with water again, P-NC was obtained and dried in vacuum (60 ℃, 8 h). The Zn atoms in sample was almost completely removed (Zn content: 0.05 wt%, by ICP-OES analysis).

Study on light response characteristics and photothermal properties. Before testing, the obtained powder samples were prepared as membranes. Briefly, 10 mg of the sample was uniformly dispersed in 100 mL of water. Then, the sample in the suspension would be tightly loaded onto a circular porous filter paper (diameter: 5 cm, average pore size: 50 μm) via vacuum filtration. After drying in the oven (60 ℃, 8 h), the sample membrane was obtained. Then, the light transmittance efficiency (T) and reflection efficiency (R) of the prepared sample were tested by the UV-Vis-NIR spectrometer (250-2500 nm). And the light absorption efficiency (A) of the sample was calculated (A = (1-T-A)×100%). The photothermal tests of all the samples were conducted in dark room only with a Xe lamp irradiation (1000 w/m^2, room

temperature: 25 ± 1 ℃, humidity: 45 ± 5 %, no wind). And the thermal infrared images were captured using the thermal infrared imager.

CO_2 cycloaddition reaction with different epoxides. Briefly, 20 mg Zn SA-NC was dispersed in the mixture containing 3 mL DMF, 0.1 mM TBAB and 0.15 mM selected epoxide in a photoreactor purged with 0.1 bar CO_2 under continuous stirring. In the reaction process, Xenon lamp was used for continuous irradiation (300 mw·cm^{-2}, 18 A, full-spectrum irradiation, 16 h) with the thermocouple temperature sensor to record the temperature changes. After the reaction, the product was separated by centrifugation (3000 rpm, 10 min). Then, 100 μL reaction product was extracted with ethyl acetate and water (1 mL:1 mL) by full shaking. After standing for 10 min, a small aliquot of the supernatant solution was detected by GC analysis with argon as a carrier gas.

Theoretical calculation details. All calculations in this work were performed using Gaussian 09 program package. Full geometry optimizations and the energies corrected by zero-point vibrational effects were performed to locate all the stationary points, using B3LYP [2]/6-31+G*.[3] The intrinsic reaction coordinate path was traced to check the energy profiles connecting each transition state to two associated minima of the proposed mechanism.[4, 5]

Characterization. The morphologies of the materials were characterized by the field-emission electron microscopy (FE-SEM, Gemini SEM, ZEISS), transmission electron microscope (TEM) and high-resolution TEM (HRTEM, JEM 2100F, JEOL). X-ray diffractometer (XRD, D8, Bruker), X-ray photoelectron spectroscopy (XPS, Thermo

Scientific, K-Alpha, Thermo Fisher) and Raman (DXR, Thermo Fisher) were used to analysis the internal structures of the prepared samples. To confirm the loading of Zn single atoms and their corresponding fine coordination structure. The aberration-corrected high-angle annular dark0field scanning transmission electron microscopy (AC-HAADF-STEM) images were acquired on JEM-ARM300F. And the X-ray absorption spectra (XAS) including X-ray absorption near-edge structure (XANES) and extended X-ray absorption fine structure (EXAFS) of the sample was collected at the Beamline of TLS07Al in National Synchrotron Radiation Research Center (NSRRC), Taiwan. The electron paramagnetic resonance (EPR, EMXPLUS, Bruker) was used to detect the photogenerated electrons. The weight change during pyrolysis was recorded by thermogravimetric analysis (TG, 1100L, METTLER TOLEDO). The thermal infrared images were captured using the combination of a thermal infrared imager (FILIR ONE PRO, FILIR) and a mobile phone (iPhone 8 plus, Apple). The optical properties of the samples were studied by the UV-Vis-NIR spectrometer (UV 3600 plus, SHIMADZU). The specific surface area and pore size of the samples were analyzed by the automatic volumetric adsorption equipment (BET, ASAP2460, Micromeritics).

Part Ⅱ. Supplementary Figures

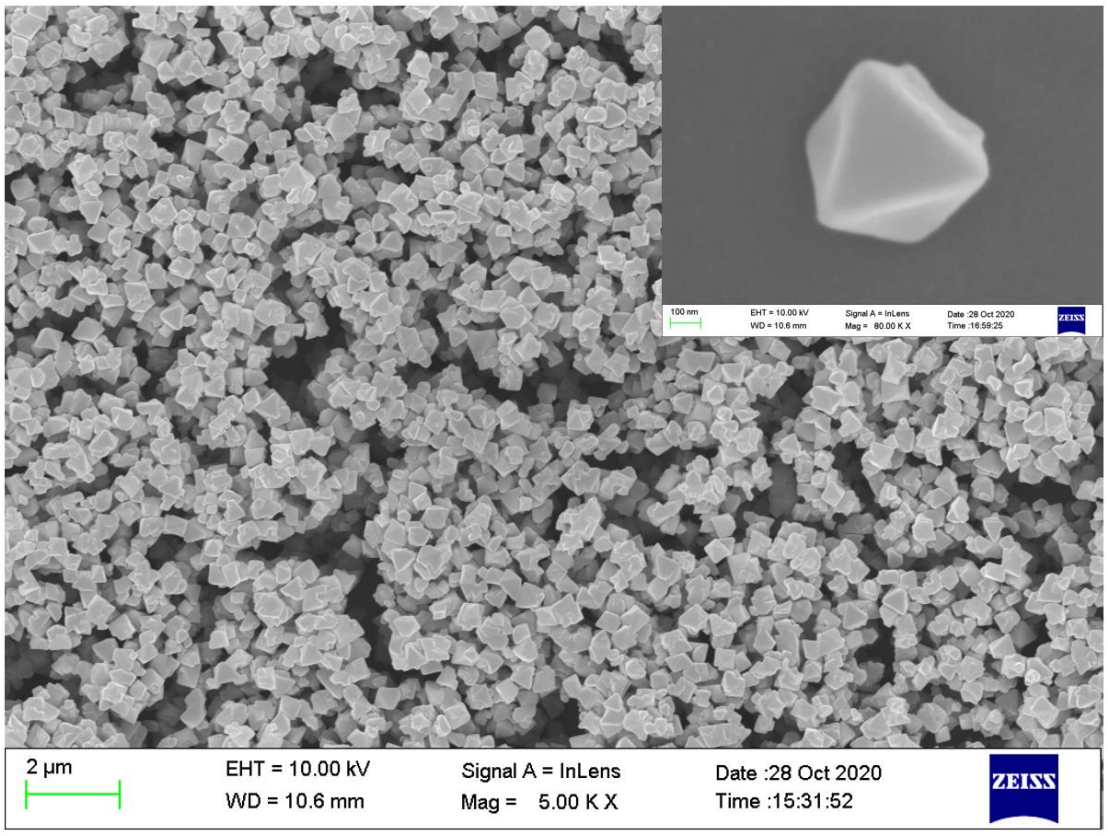


Fig. S1 SEM images of the prepared MET-6.

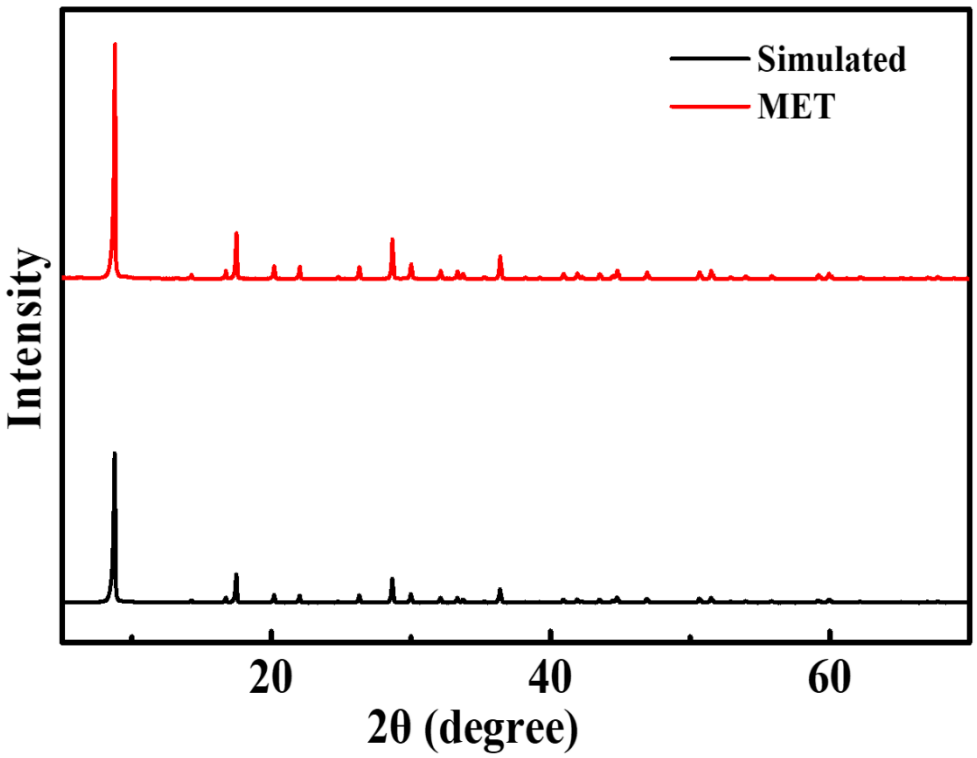


Fig. S2 XRD analysis of the prepared MET-6 and its corresponding simulated curve.

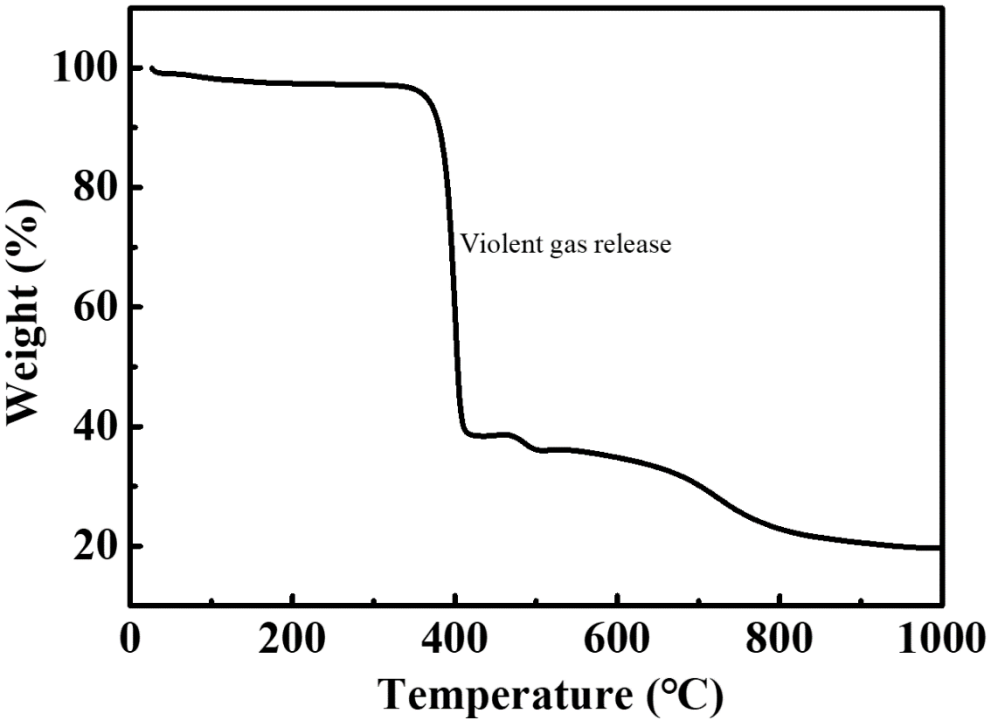


Fig. S3 TG curve of the prepared MET-6 under Ar atmosphere.

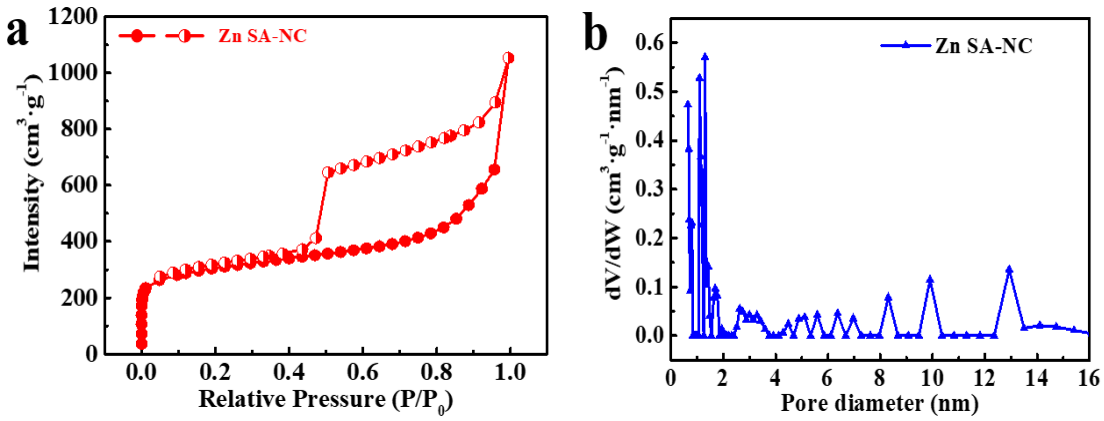


Fig. S4 N_2 adsorption/desorption test (a) and its corresponding pore size distribution curve (b).

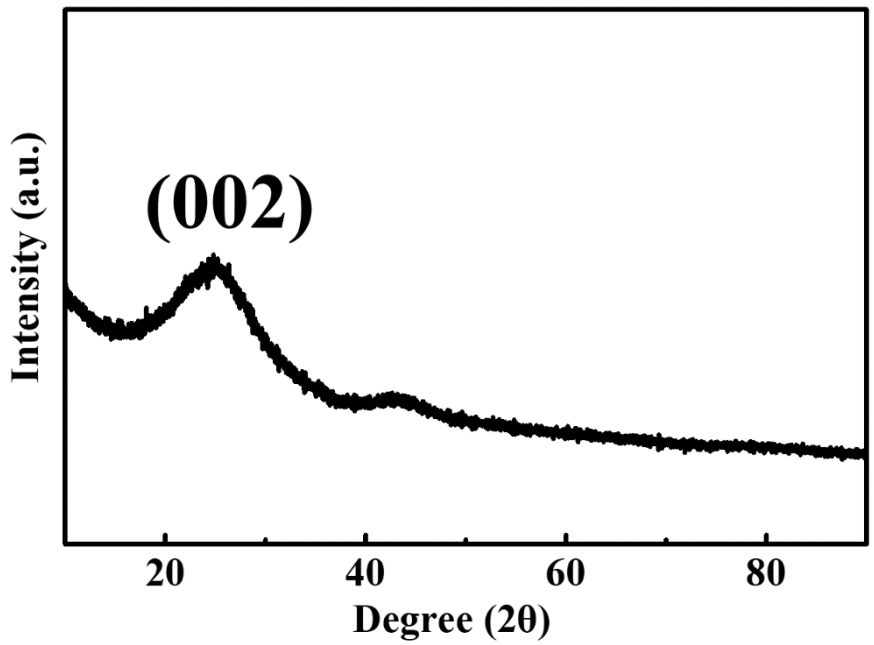


Fig. S5 XRD pattern of Zn SA-NC.

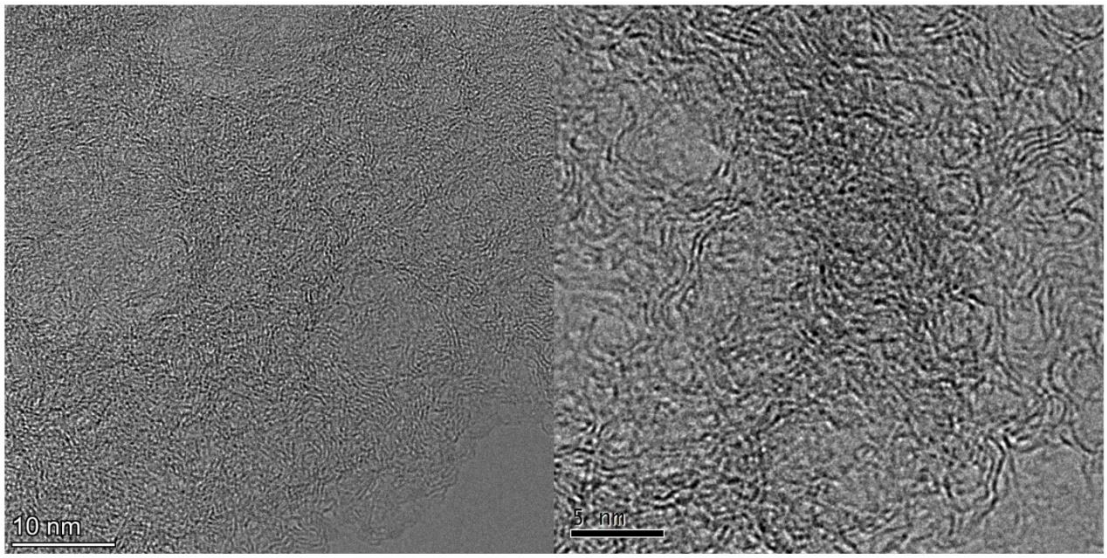


Fig. S6 HRTEM images of Zn SA-NC.

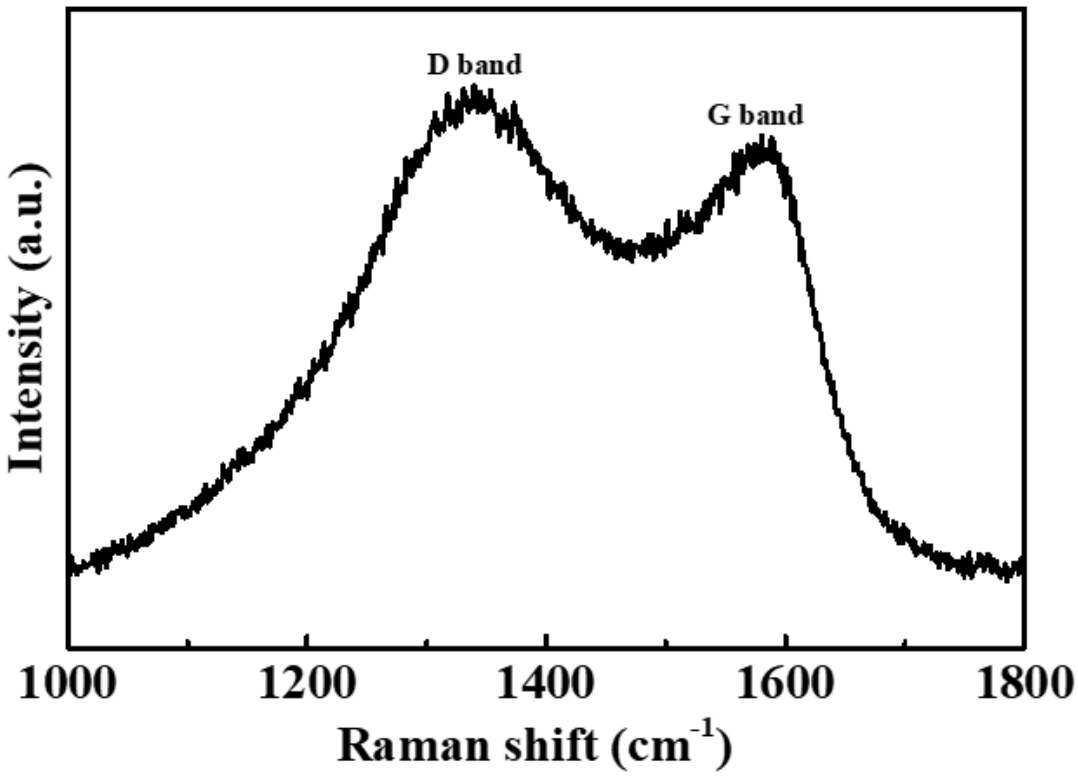


Fig. S7 Raman spectra of Zn SA-NC.

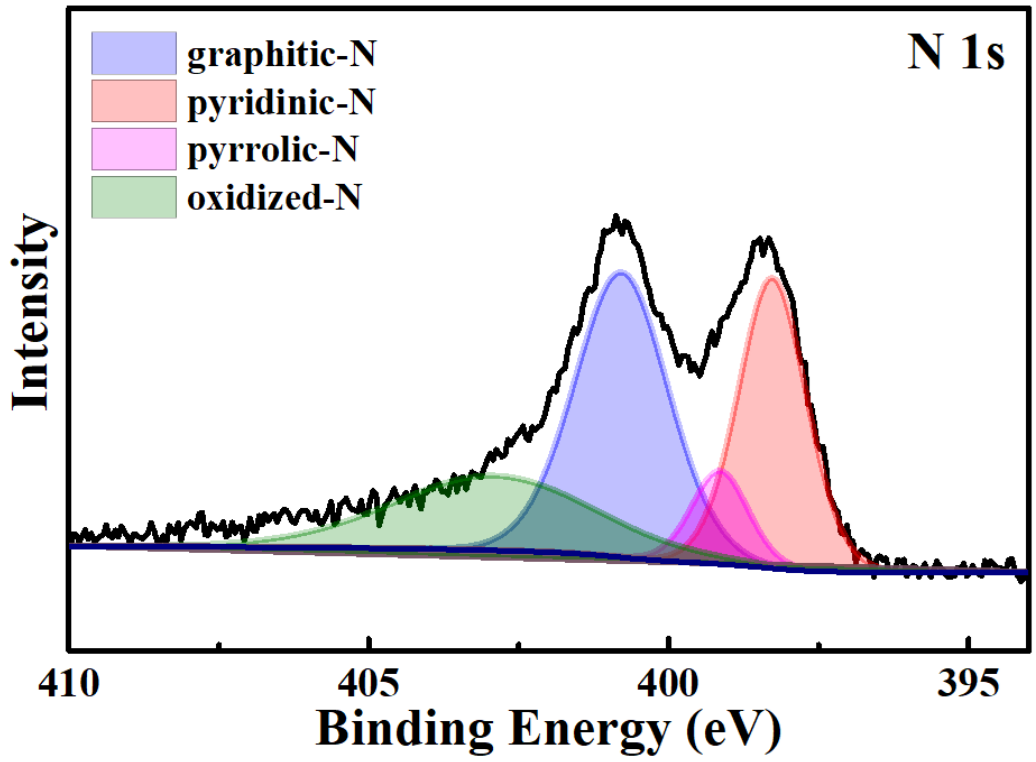


Fig. S8 High-resolution N 1s XPS spectra of Zn SA-NC.

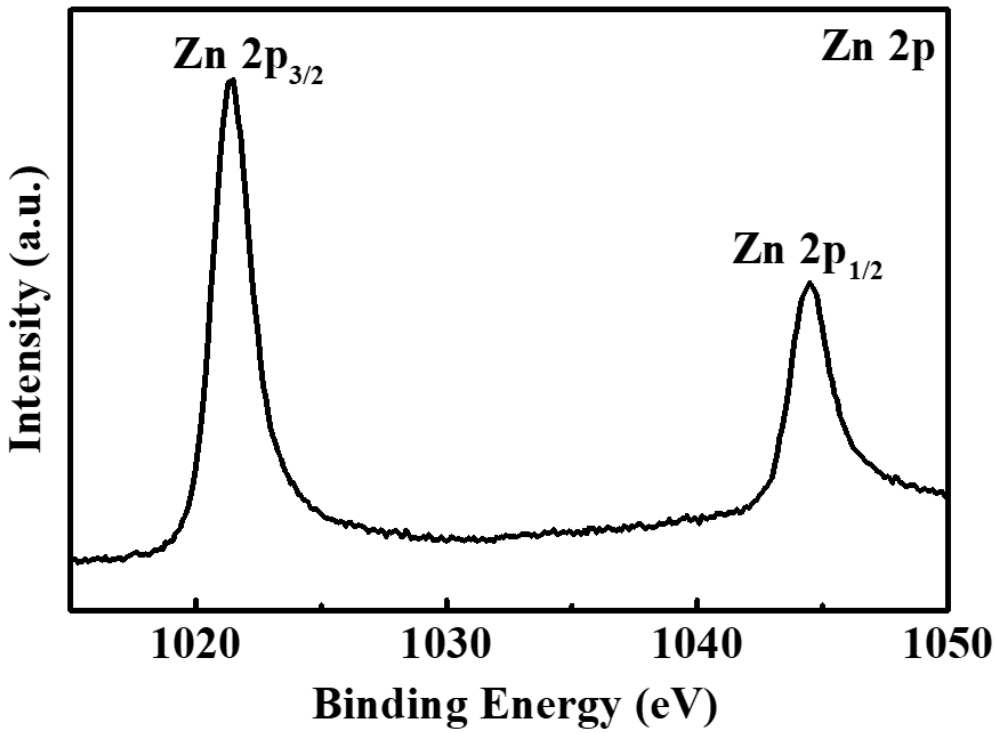


Fig. S9 High-resolution Zn 2p XPS spectra of Zn SA-NC.

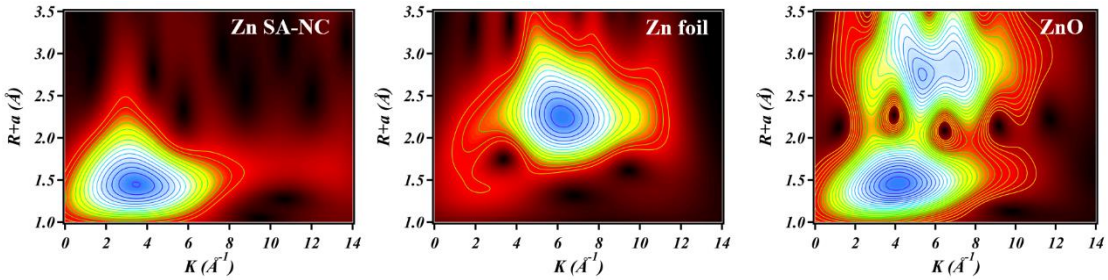


Fig. S10 Wavelet transformed-EXAFS of Zn SA-NC, Zn foil and ZnO.

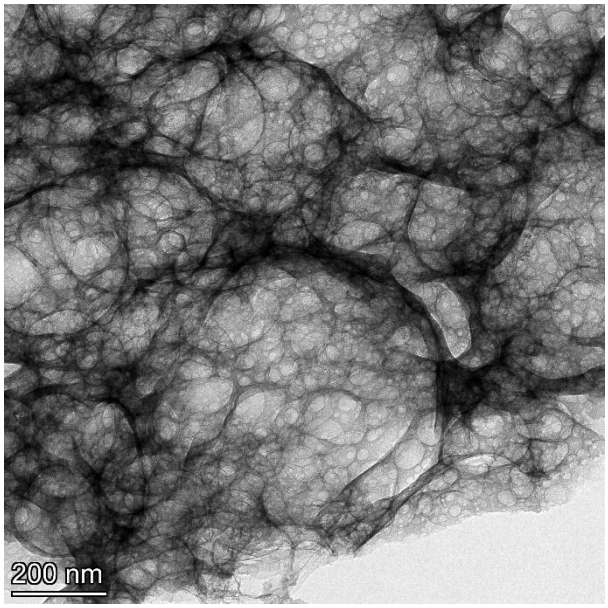


Fig. S11 TEM image of P-NC.

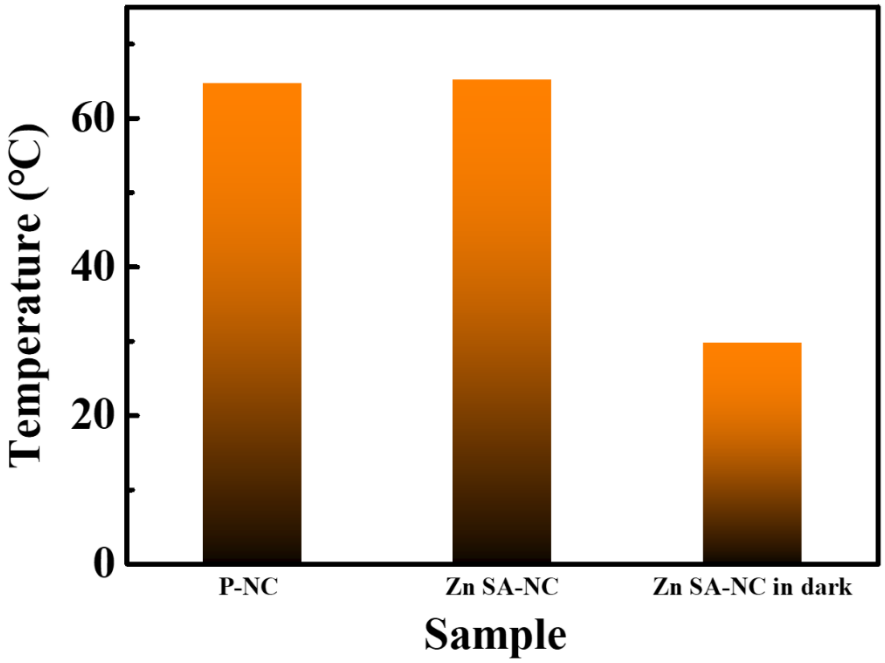


Fig. S12 Equilibrium temperature of the CO_2 cycloaddition reaction system under light irradiation.

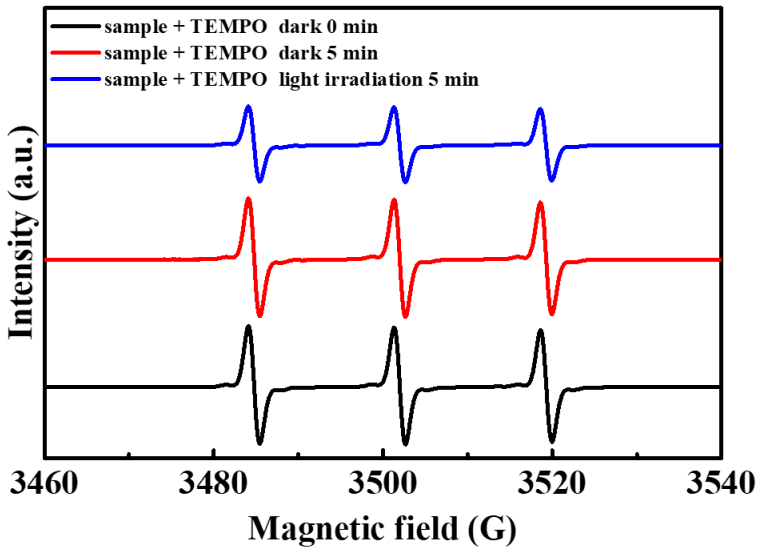


Fig. S13 Electron paramagnetic resonance (EPR) spectra of Zn SA-NC.

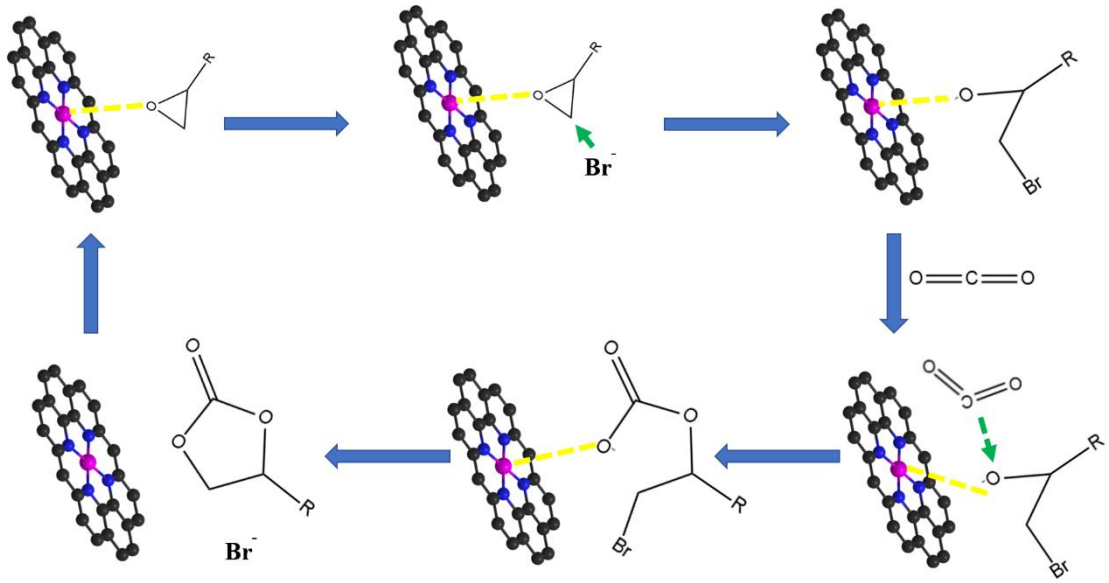


Fig. S14 Proposed mechanism for CO_2 cycloaddition with epoxides catalyzed by Zn-SA-NC.

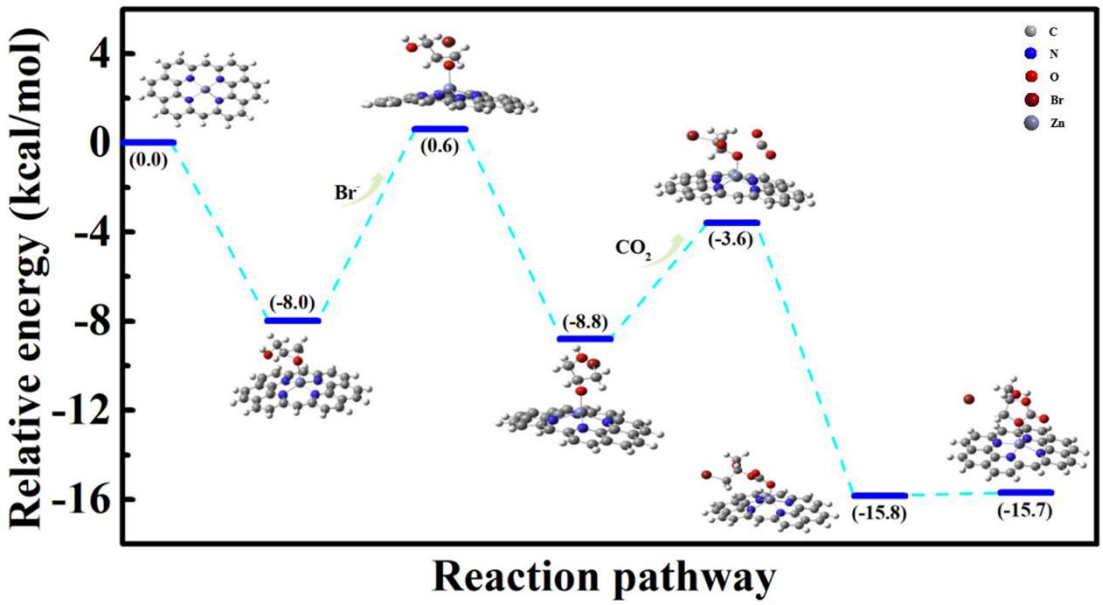


Fig. S15 Relative energy for each step of CO_2 cycloaddition by single Zn sites.

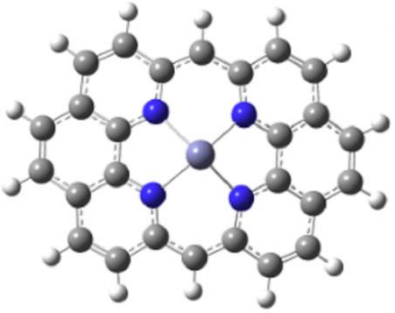
Part Ⅲ. Theoretical Calculations Results

Table S1. EXAFS fitting parameters at the Zn K-edge for various samples

Sample	Path	*N*	Δ*E*(eV)	100×*R*(Å)	$10^{-3}\times\sigma^2$(Å^2)	*R*-factor
Zn-foil	Zn-Zn1	6	-1.82(0.35)	264.4(0.5)	6.55(1.12)	0.002
	Zn-Zn2	6	-4.32(0.28)	311.3(1.1)	5.15(1.16)	
ZnO	Zn-O	4	4.11(0.69)	196.6(0.6)	2.90(0.35)	0.006
	Zn-Zn	12	6.15(0.74)	323.2(0.8)	6.25(1.22)	
Zn SA-NC	Zn-N	4.12(0.31)	5.54(0.69)	199.1(1.2)	7.57(1.34)	0.006

N: coordination numbers; *R*: bond distance; σ^2: Debye-Waller factor; Δ*E*: the inner potential correction; *R*-factor: goodness of fit.

Geometry structures:



C	-3.47743	2.51896	-0.00447
C	-2.7004	1.29635	0.00251
C	-0.72679	2.66852	-0.00172
C	-1.43277	3.88346	-0.01075
C	-2.86533	3.75074	-0.01122
C	0.72584	2.66937	-0.00124
C	2.70104	1.29964	0.00395
C	3.47661	2.52277	0.00454
C	2.86308	3.75394	0.0013
C	1.43034	3.8852	-0.00447
C	0.68937	5.10963	-0.01372
C	-0.69334	5.10865	-0.01805
H	-1.2376	6.04987	-0.02672
H	1.23283	6.05161	-0.01877
H	-4.56201	2.45163	-0.00462
H	-3.47455	4.65197	-0.01713
H	4.56129	2.45627	0.00744
H	3.47172	4.65588	0.0026
N	1.35574	1.46496	0.00212
N	-1.35506	1.46394	0.00669
Zn	0.	0.	0.01896
C	-3.47661	-2.52277	0.00454
C	-2.70104	-1.29964	0.00395
C	-0.72584	-2.66937	-0.00124
C	-1.43034	-3.8852	-0.00447
C	-2.86308	-3.75394	0.0013
C	0.72679	-2.66852	-0.00172
C	2.7004	-1.29635	0.00251
C	3.47743	-2.51896	-0.00447
C	2.86533	-3.75074	-0.01122
C	1.43277	-3.88346	-0.01075
C	0.69334	-5.10865	-0.01805
C	-0.68937	-5.10963	-0.01372
H	-1.23283	-6.05161	-0.01877
H	1.2376	-6.04987	-0.02672
H	-4.56129	-2.45627	0.00744

H	-3.47172	-4.65588	0.0026
H	4.56201	-2.45163	-0.00462
H	3.47455	-4.65197	-0.01713
N	1.35506	-1.46394	0.00669
N	-1.35574	-1.46496	0.00212
C	-3.30579	-0.00134	0.00452
H	-4.39232	-0.00112	0.00422
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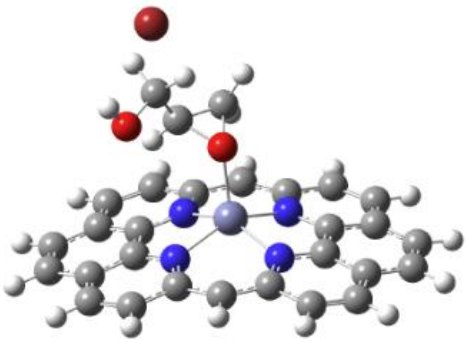
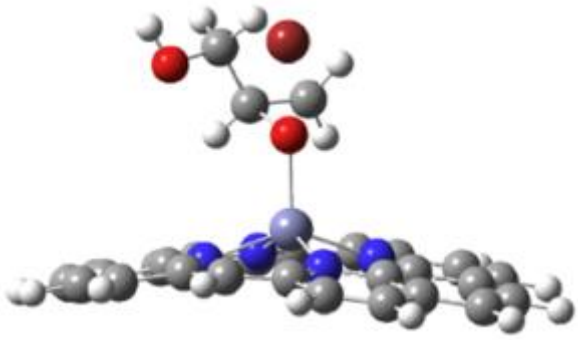
H	4.39232	0.00112	0.00422



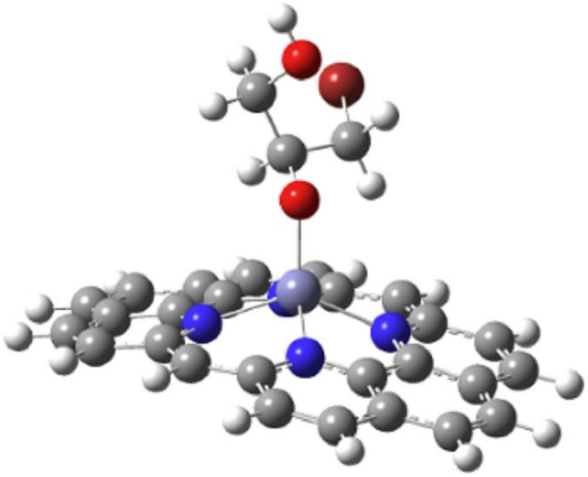
O	0.65593	0.77609	-1.91736
C	2.11923	0.66459	-2.03455
H	2.57487	0.15161	-1.19111
C	1.51538	1.96661	-1.79143
H	1.39557	2.66587	-2.61341
H	1.55701	2.39163	-0.79539
C	2.63495	0.28216	-3.38485
H	2.04515	0.77791	-4.16746
H	3.67503	0.62852	-3.45607
O	2.55852	-1.14415	-3.51186
H	2.993	-1.39546	-4.34398
Br	4.6217	3.2999	-1.34782
C	0.08621	-4.28652	-0.49391
C	-0.52565	-2.97628	-0.54293
C	1.34698	-2.14243	0.67942
C	1.96483	-3.40222	0.79728
C	1.28543	-4.48427	0.14283
C	1.91645	-0.99417	1.35073
C	1.59582	1.29269	1.94993
C	2.81709	1.21274	2.72114
C	3.53387	0.04544	2.79277
C	3.08627	-1.14119	2.12038
C	3.71417	-2.42265	2.19566
C	3.17057	-3.51827	1.55522
H	3.64965	-4.49144	1.63215
H	4.62484	-2.52611	2.7809
H	-0.43317	-5.12229	-0.95508
H	1.72369	-5.47924	0.17848
H	3.15059	2.09402	3.26241
H	4.44525	0.00316	3.38502
N	1.24926	0.18747	1.24155
N	0.18662	-1.95322	-0.00556
Zn	-0.27746	0.03406	-0.12139
C	-4.0584	-1.68941	-1.40606
C	-2.66649	-1.63447	-1.01358

C	-3.0405	0.61177	-0.29544
C	-4.41024	0.59962	-0.62094
C	-4.88882	-0.61268	-1.22339
C	-2.46694	1.76162	0.36992
C	-0.5386	2.63865	1.46796
C	-1.3143	3.81873	1.78431
C	-2.62705	3.92673	1.40053
C	-3.28152	2.86509	0.68924
C	-4.6608	2.84379	0.31616
C	-5.20791	1.74594	-0.31771
H	-6.26221	1.73615	-0.58385
H	-5.28114	3.70489	0.55328
H	-4.44351	-2.61152	-1.83303
H	-5.93445	-0.67795	-1.51625
H	-0.84231	4.61618	2.35188
H	-3.19612	4.81776	1.6567
N	-1.15063	1.69509	0.70755
N	-2.21759	-0.44547	-0.53452
C	-1.83105	-2.78679	-1.08353
H	-2.29538	-3.67483	-1.50385
C	0.78211	2.46249	1.97253
H	1.17621	3.29407	2.5504



O	0.92293	-1.50534	0.36922
C	0.70674	-2.73947	0.93557
H	0.21926	-2.65733	1.9333
C	2.25873	-2.6688	0.94154
H	2.74708	-2.82209	-0.01952
H	2.88639	-1.97081	1.49682
C	-0.1981	-3.68591	0.13415
H	0.30673	-3.98202	-0.79637
H	-0.38829	-4.59099	0.73347
O	-1.41772	-3.02824	-0.16926
H	-2.00926	-3.67624	-0.58183
Br	2.39703	-4.68978	2.05738
C	-2.6945	0.06042	-3.5199
C	-1.51319	0.31623	-2.72794
C	-2.84831	0.19229	-0.77745
C	-4.05253	0.03539	-1.50273
C	-3.91654	-0.08872	-2.92285
C	-2.88569	0.38229	0.65713
C	-1.69341	1.15117	2.54644
C	-2.94532	1.22502	3.26969
C	-4.12285	0.88346	2.66694
C	-4.14354	0.50133	1.28507
C	-5.34595	0.30319	0.53768
C	-5.30231	0.04991	-0.81513
H	-6.2184	-0.08624	-1.38622
H	-6.30134	0.36547	1.05383
H	-2.60042	0.02368	-4.60263
H	-4.80475	-0.25137	-3.52971
H	-2.93033	1.60259	4.28929
H	-5.06178	0.94325	3.21251
N	-1.69453	0.54907	1.32555
N	-1.63551	0.26645	-1.37888
Zn	-0.13133	0.19399	0.04693
C	1.96816	1.65074	-3.63963
C	0.89	1.15905	-2.80489

C	2.06481	1.95111	-0.92311
C	3.15373	2.44904	-1.66956
C	3.06649	2.25318	-3.08527
C	1.98876	2.22163	0.49273
C	0.67154	2.08466	2.43775
C	1.67803	2.8487	3.13949
C	2.82006	3.25404	2.50297
C	3.0239	2.95015	1.12121
C	4.15192	3.37736	0.3548
C	4.21283	3.13859	-1.00164
H	5.07521	3.46384	-1.57966
H	4.95984	3.9026	0.86044
H	1.8801	1.5479	-4.71864
H	3.88013	2.60041	-3.71806
H	1.49319	3.12426	4.1757
H	3.57876	3.82216	3.03754
N	0.8596	1.82105	1.12158
N	1.03562	1.25732	-1.46225
C	-0.28885	0.6271	-3.38148
H	-0.30193	0.56773	-4.46605
C	-0.51627	1.68896	3.11713
H	-0.58915	1.99716	4.15609



O	-2.22285	-1.49935	0.08032
C	-1.25221	-0.68812	-0.41218
H	-0.85822	-1.00541	-1.41662
C	-0.08139	-0.79399	0.57472
H	-0.30154	-0.32639	1.5335
H	0.21244	-1.83425	0.70338
C	-1.66802	0.77842	-0.63698
H	-0.86644	1.32307	-1.15794
H	-2.56316	0.77889	-1.27763
O	-1.95995	1.43515	0.61125
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Br	1.65629	0.09792	-0.04259
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C	-6.20267	-2.60396	0.10094
C	-5.24739	-2.94745	-2.05534
C	-6.40851	-2.55164	-2.74797
C	-7.49559	-2.10505	-1.92408
C	-4.11402	-3.4688	-2.78756
C	-1.98488	-4.52472	-2.62406
C	-1.97939	-4.63499	-4.06661
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C	-4.18018	-3.58369	-4.18998
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C	-6.43499	-2.64069	-4.17373
H	-7.32939	-2.32016	-4.70295
H	-5.39212	-3.22103	-5.95635
H	-8.248	-1.8292	0.05674
H	-8.41118	-1.76155	-2.40066
H	-1.12836	-5.10818	-4.54923
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N	-5.15171	-2.91842	-0.69895

Zn	-3.22082	-3.31229	-0.08169
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C	-5.15637	-3.43168	2.29162
C	-3.0958	-4.62023	2.43817
C	-3.27632	-4.97724	3.78881
C	-4.46616	-4.46623	4.40719
C	-1.95056	-5.11954	1.7086
C	-0.91857	-5.31502	-0.43004
C	0.08589	-6.15769	0.18233
C	0.03535	-6.46076	1.51922
C	-1.02778	-5.96954	2.34898
C	-1.21727	-6.29276	3.72807
C	-2.30644	-5.81121	4.42607
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H	-0.49314	-6.93852	4.21928
H	-6.2856	-3.37256	4.16352
H	-4.65214	-4.68819	5.4558
H	0.87456	-6.567	-0.44339
H	0.79363	-7.10427	1.96014
N	-1.84985	-4.77537	0.39668
N	-3.98337	-3.85088	1.75283
C	-6.15178	-2.77252	1.51415
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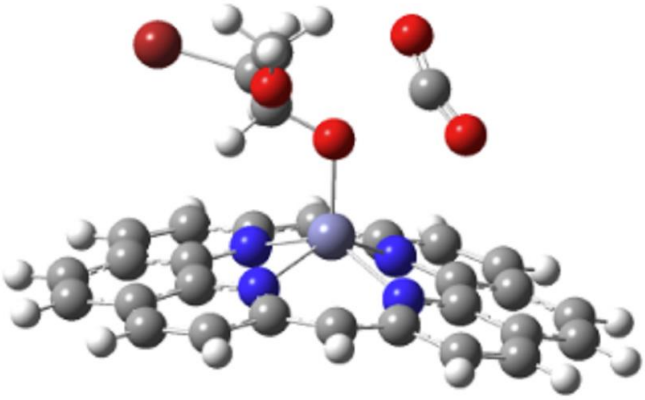

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C	-1.8383	-2.36679	-0.75257
H	-1.177 97	-3.19428	-1.00127
H	-1.60821	-1.97154	0.23414
C	-2.10624	-1.8003	-3.22332
H	-1.26109	-1.59504	-3.89456
H	-2.23478	-2.88642	-3.14881
O	-3.29391	-1.19278	-3.76383
H	-3.18038	-1.09666	-4.72117
Br	-3.66167	-3.18922	-0.50508
C	0.32514	4.52955	-1.65107
C	0.85528	3.25452	-1.21843
C	-1.12803	2.93876	0.0522
C	-1.67673	4.19024	-0.29696
C	-0.8956	4.97274	-1.21036
C	-1.81708	2.092	1.0023
C	-1.69397	0.12318	2.3269
C	-2.96434	0.48905	2.91447
C	-3.60812	1.6414	2.54355
C	-3.0294	2.52764	1.57559
C	-3.57875	3.78708	1.18225
C	-2.92359	4.59272	0.27367
H	-3.34437	5.55456	-0.0107
H	-4.52099	4.10753	1.62087
H	0.92321	5.14349	-2.31958
H	-1.27504	5.93902	-1.53604
H	-3.39286	-0.15829	3.67524
H	-4.55835	1.90749	3.0018
N	-1.22057	0.9157	1.3311
N	0.06178	2.49121	-0.42566
Zn	0.31531	0.4398	-0.0277
C	4.34676	1.64553	-1.31171

C	2.92952	1.7652	-1.04612
C	3.11726	-0.09459	0.42148
C	4.50839	-0.23216	0.2383
C	5.10034	0.67683	-0.69989
C	2.43296	-0.92942	1.38507
C	0.39059	-1.34695	2.52153
C	1.07296	-2.36358	3.29112
C	2.40586	-2.62043	3.09544
C	3.16374	-1.87496	2.13357
C	4.56751	-2.0174	1.90491
C	5.21942	-1.22107	0.98623
H	6.29039	-1.32744	0.82905
H	5.11913	-2.75854	2.47891
H	4.8112	2.35307	-1.99373
H	6.16667	0.60522	-0.90407
H	0.51295	-2.91078	4.0451
H	2.90801	-3.38209	3.68836
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N	2.37023	0.82746	-0.23979
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H	2.71672	3.53056	-2.22492
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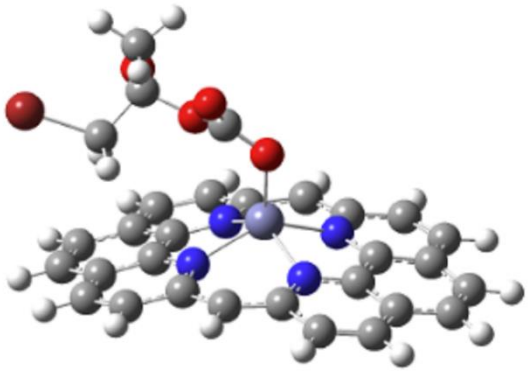

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H	3.79851	2.27984	1.65583
H	3.1045	0.80674	0.90653
C	4.25633	3.67286	-0.70651
H	5.27175	3.37108	-0.99459
H	3.81986	4.24733	-1.53414
O	4.29673	4.45883	0.4916
H	4.82918	5.25095	0.31236
Br	5.59235	0.85227	0.62829
C	1.05458	1.89737	-0.84942
O	0.47138	1.28596	0.06863
O	0.90454	1.84431	-2.09002
C	-3.25677	0.46568	3.70776
C	-2.29097	-0.1437	2.81874
C	-3.39041	0.93952	1.00272
C	-4.38741	1.51649	1.8137
C	-4.25663	1.26886	3.22139
C	-3.46086	1.07956	-0.43531
C	-2.54519	0.39316	-2.52464
C	-3.59945	1.13678	-3.17941
C	-4.54532	1.81238	-2.45216
C	-4.5305	1.78751	-1.01756
C	-5.50969	2.39358	-0.17183
C	-5.43971	2.26364	1.20062
H	-6.19821	2.71823	1.83371
H	-6.32392	2.95077	-0.62916
H	-3.19034	0.25707	4.77223
H	-4.98103	1.70905	3.90322
H	-3.63895	1.13717	-4.26547
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N	-2.37135	0.19238	1.50581

Zn	-0.97924	-0.24528	0.04466
C	0.24366	-3.02161	3.18137
C	-0.48812	-1.94758	2.5455
C	0.32107	-2.73972	0.4484
C	1.01626	-3.82918	1.00881
C	0.96978	-3.91881	2.44027
C	0.26847	-2.58196	-0.98879
C	-0.71293	-1.37998	-2.79685
C	-0.04772	-2.29076	-3.70349
C	0.73561	-3.31279	-3.23071
C	0.90286	-3.52482	-1.82106
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C	1.68244	-4.75151	0.14409
H	2.22649	-5.58357	0.5849
H	2.1254	-5.32069	-1.87618
H	0.19338	-3.11776	4.26273
H	1.5057	-4.72566	2.93549
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N	-0.35769	-1.83176	1.19956
C	-1.33965	-1.08868	3.29848
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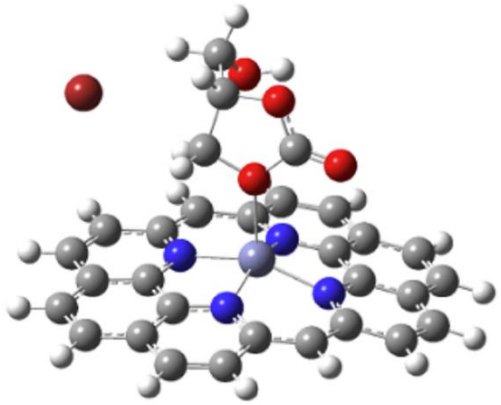

O	-1.13044	-2.37502	-3.18032
C	-2.298	-2.495	-2.29792
H	-3.18805	-2.41838	-2.92024
C	-2.14048	-1.29154	-1.36236
H	-2.267	-1.53311	-0.31183
H	-2.76465	-0.44516	-1.64199
C	-2.24308	-3.84607	-1.60568
H	-3.11132	-3.91329	-0.94506
H	-2.30364	-4.64911	-2.35094
O	-1.07615	-3.98533	-0.7927
H	-0.31947	-4.19611	-1.36626
Br	-5.4124	-1.91042	-0.7839
C	-0.23547	-1.52553	-2.66497
O	0.86901	-1.32108	-3.1038
O	-0.73998	-0.90243	-1.56866
C	-0.27973	4.37586	-1.58554
C	0.40419	3.13606	-1.28503
C	-1.44808	2.54678	0.10564
C	-2.13437	3.75564	-0.11483
C	-1.50053	4.66418	-1.02893
C	-1.96266	1.5876	1.05894
C	-1.52442	-0.44074	2.24252
C	-2.75791	-0.22658	2.96749
C	-3.53792	0.87633	2.72796
C	-3.15037	1.8646	1.76124
C	-3.84912	3.08175	1.49262
C	-3.357	3.998	0.5841
H	-3.8908	4.92753	0.40071
H	-4.77312	3.2846	2.02878
H	0.2026	5.09104	-2.24638
H	-1.99196	5.60709	-1.2585
H	-3.0507	-0.9508	3.72289
H	-4.45772	1.02262	3.28991
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C	0.67946	-1.75962	2.11633
C	1.5031	-2.79223	2.70771
C	2.82154	-2.93585	2.3546
C	3.43568	-2.05634	1.39953
C	4.81329	-2.07137	1.01885
C	5.31445	-1.14368	0.12683
H	6.36748	-1.1584	-0.14399
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H	4.35709	2.6488	-2.44157
H	5.93391	0.93142	-1.65342
H	1.06225	-3.44595	3.45548
H	3.42517	-3.71297	2.81832
N	1.26071	-1.0034	1.15056
N	2.23635	0.79989	-0.59764
C	1.72919	2.8857	-1.74793
H	2.15196	3.65627	-2.38691
C	-0.65354	-1.52326	2.56138
H	-1.01478	-2.20022	3.33079

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