Supplementary Information (SI) for Inorganic Chemistry Frontiers.

Supporting information

Boosting oxygen reduction activity on silver nanocluster via selectively exposure of solvent coordinated sites

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1. Experimental Section

1.1 Chemicals

All solvents and reagents were purchased from commercial sources and were used without further purification. Naphthalen-2-yl-methanethiol used in this work were synthesized according to literature methods.

1.2 Synthesis of $Ag_{12}(SCH_2C_{10}H_7)_6(CF_3CO_2)_6(CH_3CN)_6$

Naphthalen-2-yl-methanethiol (17 mg, 0.100 mmol) and $AgCF_3CO_2$ (44 mg, 0.200 mmol) were dissolved in 3 mL acetonitrile and 3 mL acetone at room temperature. The solution turned to nearly translucent after stirred 3-5 min. The mixed solution was kept under a dark environment for 1 days to afford pale yellow crystals. The crystals (named AgNCs) were filtered and washed with diethyl ether. (yield: 68 % based on ligand).

1.3 Synthesis of AgNCs@GO

AgNCs@GO was synthesized by photodeposition method. AgNCs (1mg) and GO (10mg) were mixed in 50mL dichloromethane with ultrasonic dispersion for 10 min before subjected to the irradiation. After 30 min, the mixture was centrifuged for 2 min at 10000 r/min. Then the catalyst was washed with dichloromethane and dried thoroughly at room temperature.

1.4 Characterization

X-ray diffraction (XRD) patterns were measured by Riguku D/Max-2500PC X-ray diffractometer with Cu sealed tub (λ = 1.54178 Å). Field-emission scanning electron microscopy (FESEM) images were obtained using Zeiss Sigma 500. Transmission electron microscopy (TEM) and high-resolution transmission electron microscopy (HRTEM) images were collected using FEI TalosF200S at an accelerating voltage of 200 kV. X-ray photoelectron spectroscopy (XPS) were performed on a Thermo ESCALAB 250XI electron spectrometer using 300 W Al K radiation. Inductively coupled plasma mass spectrometry (ICP-MS) were performed on ICPE-9820. UV–vis absorption spectra were recorded with a U-2000 spectrophotometer. Solid-state UV–vis absorption spectra were measured from 200 to 800 nm using barium sulfate (BaSO4) as a standard on a TU-1901 double-beam UV–vis spectrophotometer.

1.5 Electrochemical Measurements

All catalysts electrochemical performances were carried out in a conventional three-electrode cell using CHI 760E electrochemical workstation. Rotating disk electrode (RDE, 0.197 cm^2) was used as working electrode, saturated Ag/AgCl electrode was used as reference electrode, Pt wire was used as counter electrode, respectively. The catalyst ink was prepared by dispersing 2 mg of catalyst and 3 mg of VXC-72R in 360 µL of DMF and 40 µL of 5 wt% nafion. Finally, 10 µL of the catalyst ink was dropped onto the RDE electrode.

Firstly, cyclic voltammetry (CV) tests were conducted in N_2 and O_2 saturated 0.1 M KOH solution from -1 V to 0.2 V with a scan rate of 50 mV s^{-1}. The RDE tests were performed at various rotating speeds ranging from 400 to 2500 rpm with a sweep rate of 5 mV s^{-1}. RRDE measurements were conducted by liner sweep voltammetry (LSV) from -1 V to 0.2 V at 5 mV s^{-1} with a rotating speed of 1600 rpm using high potential (1.0 V vs RHE) on the platinum ring electrode.

All testing data were converted to reversible hydrogen electrode (RHE) via Nernst equation: $E_{RHE} = E_{Ag/AgCl} + (0.197 + 0.0592\ pH)$ before analyzing.

The electron transfers number (n) was respectively calculated by the following equations.

From RRDE analysis:

$$n = \frac{4I_D}{I_R/N + I_D}$$

Where n is the electron transfer number, I_d is the disk current, *Ir* is the ring current and *N* is the current collection efficiency (0.37) of the Pt ring of RRDE electrode.

From Koutecky-Levich (K-L) analysis:

$$\frac{1}{J} = \frac{1}{J_L} + \frac{1}{J_K} = \frac{1}{B\omega^{0.5}} + \frac{1}{J_K}$$

$$B = 0.62nFC_0(D_0)^{2/3}v^{-1/6}$$

Where J is the measured current density, J_K and J_L are the kinetic and diffusion-limited current densities. respectively, B is determined from the slope of the Koutechy-Levich

(K-L) plot based on Levich equation. ω is electrode rotation rate, F is the faraday constant (96485 C mol^{-1}), D_{O2} is the diffusion coefficient of O_2 (1.90×10^{-5} cm^2 s^{-1}), C_0 is the bulk concentration of O_2 (1.2×10^{-6} $mol\cdot cm^{-3}$), and v is the kinetic viscosity (v=0.01009cm^2 s^{-1}). The constant 0.62 is adopted when the rotation speed is expressed in rad s^{-1}.

1.6 Computation methods.

Computational Details

The Vienna ab-initio simulation package (VASP)[1-2] based on density functional theory (DFT) is employed in theoretical calculation. The generalized gradient approximation (GGA) calculation was performed with the Perdew–Burke–Ernzerhof (PBE) exchange-correlation potential.[3] A plane-wave cutoff energy of 400 eV was used. The Fermi scheme was employed for electron occupancy with an energy smearing of 0.1 eV. The first Brillouin zone was sampled in the Monkhorst-Pack grid[4] with k-point mesh of 3×3×1. The energy (converged to 1.0 ×10 -6 eV/atom) and force (converged to 0.01eV/Å) were set as the convergence criterion for geometry optimization. All calculations were spin-polarized.

The ORR performed on Ag site was calculated by the following theory.

(i) O_2 (g) + * → O_2*

(ii) * + O_2 (g) + H_2O(l) + e^- → OOH* + OH

(iii) OOH * + e^- → O* + OH

(iv) O* + $2H^+$ + $2e^-$ + H_2O → *OH + OH

(v) *OH + e^- → * + OH

Overall reaction:

O_2 (g) + H_2O(l) + $4e^-$ → $4OH^-$

where * represents an active site on the corresponding surface.

The electrocatalyst is working under a potential in reality. To investigate the effects of the electric potential on the activity of ORR, the free energy diagrams of ORR[5] is employed. Free energy change from initial states to final states of the reaction is calculated as follows:

$\Delta G = \Delta E + \Delta ZPE - T\Delta S + \Delta G_U + \Delta G_{pH}$

where ΔE is the energy difference of reactants and products, ΔZPE and ΔS is the change in zero-point energy and in entropy, respectively, T is room temperature (298.15 K). $\Delta G=-eU$, here U is the potential at the electrode and e is the transferred charge. ΔG_{pH} is the correction of the H^+ free energy. The free energy of H + ions has been corrected by the concentration dependence of the entropy:

$\Delta G_{pH} = -kT\ln[H^+] = kT\ln10\times pH$

(0.773844 for 0.1M KOH).

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2. Supplementary Figures and Tables

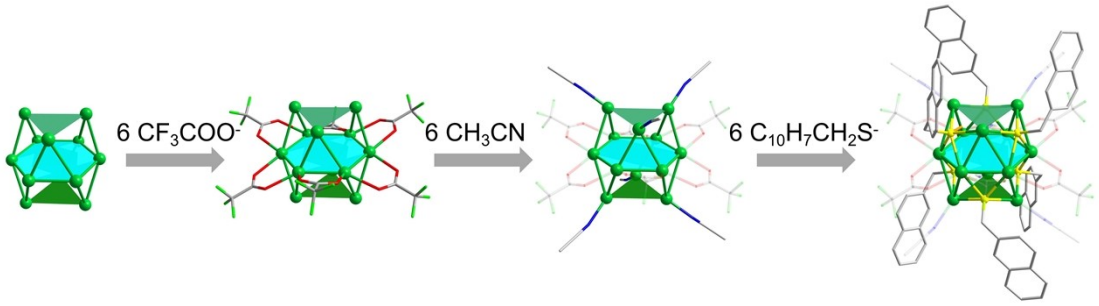

Figure S1. The structure and coordination mode of AgNCs.

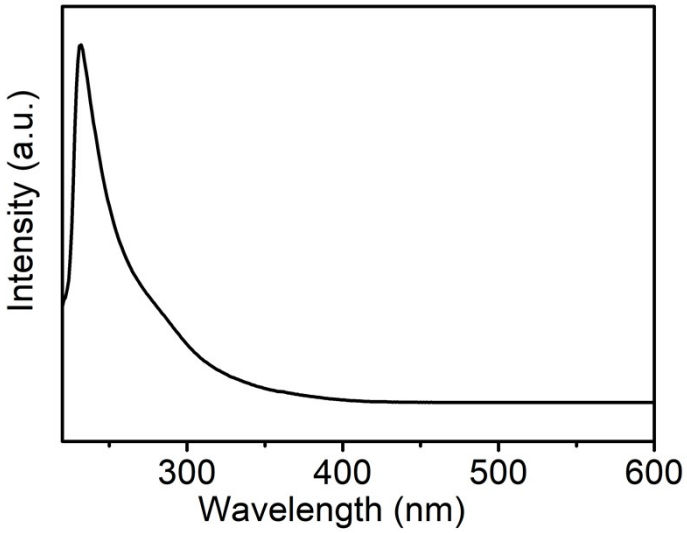

Figure S2. UV/Vis absorbance spectra of AgNCs.

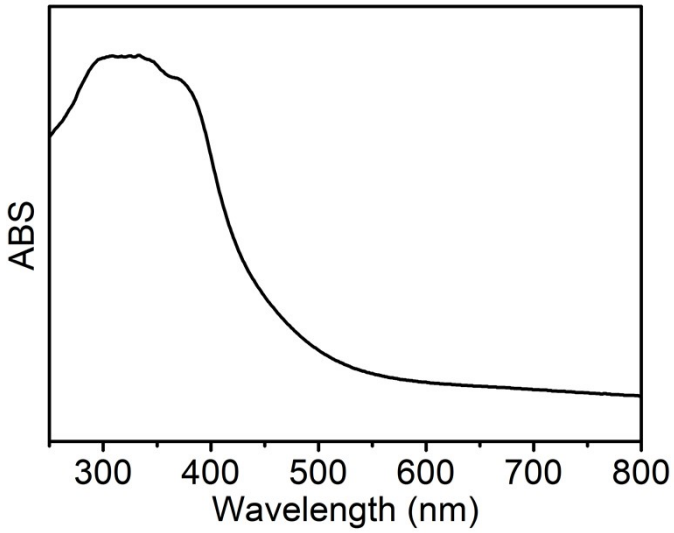

Figure S3. Solid state diffuse reflectance spectrum of AgNCs.

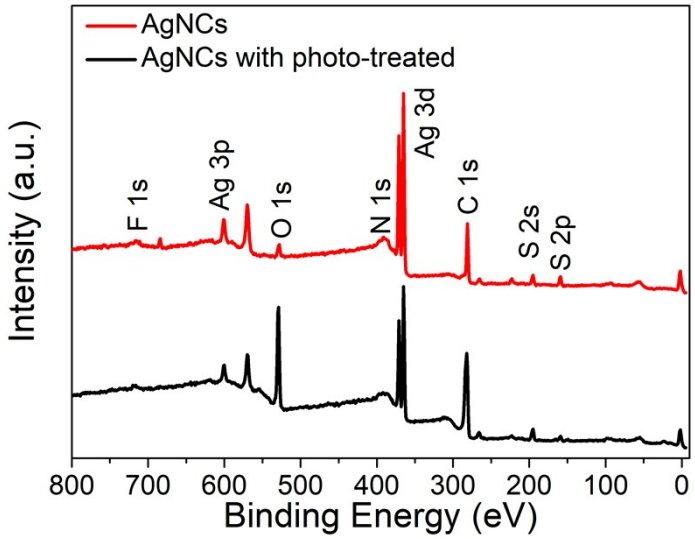

Figure S4. XPS survey spectrum of AgNCs and AgNCs with photo-treated.

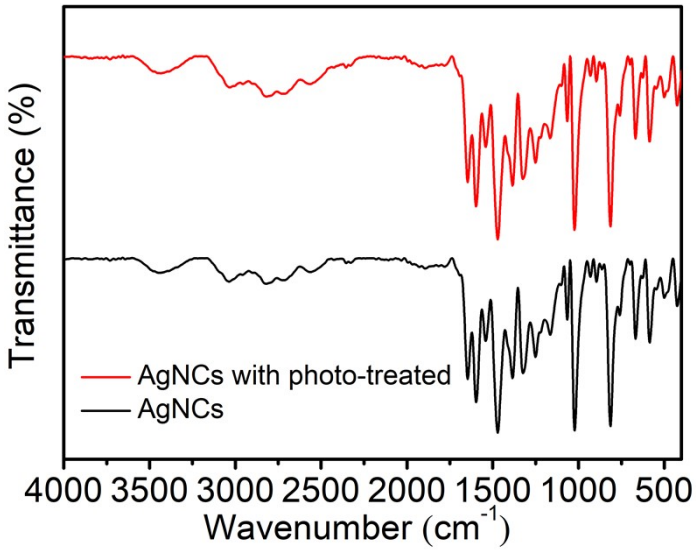

Figure S5. FT-IR spectra of AgNCs and AgNCs with photo-treated.

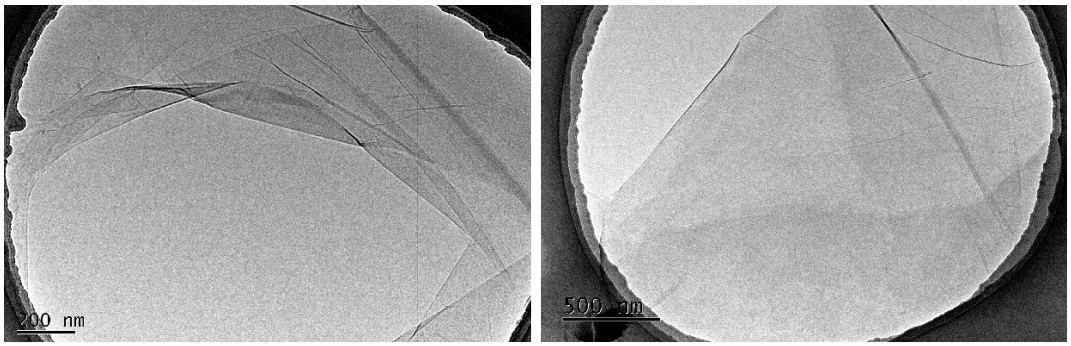

Figure S6. TEM images of GO.

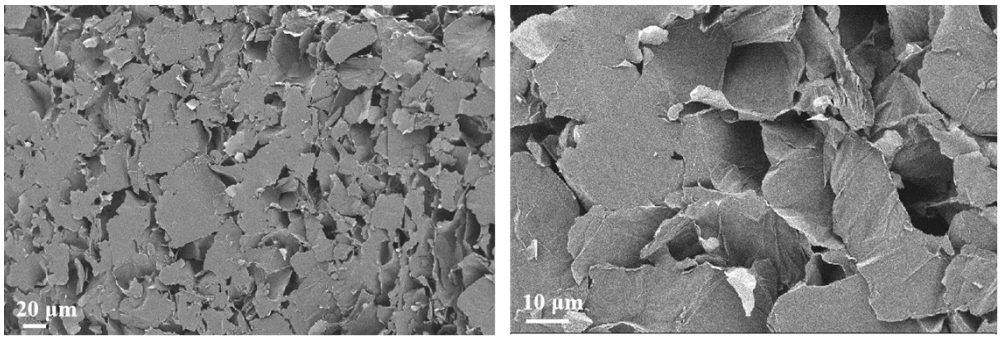

Figure S7. SEM images of AgNCs@GO.

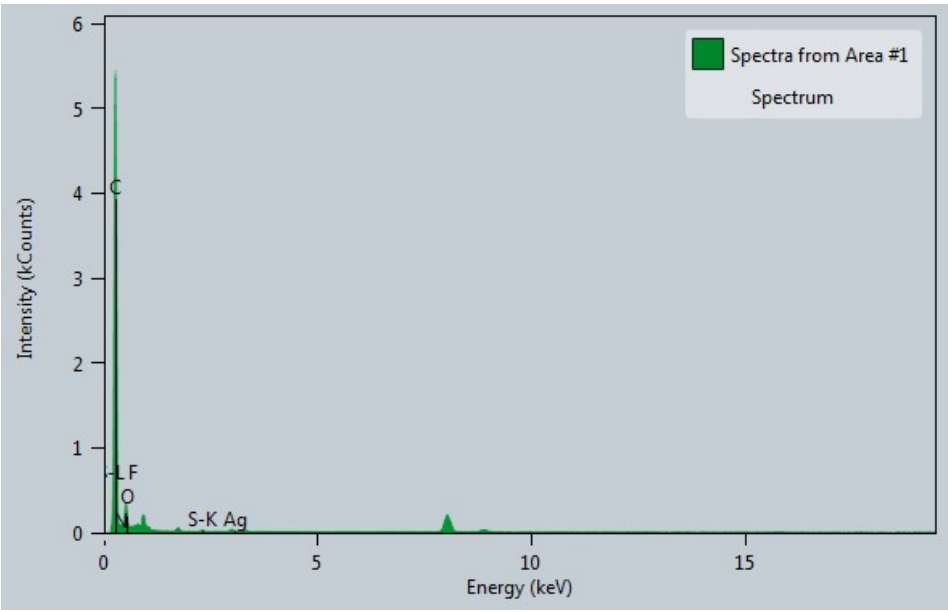

Figure S8. EDS elemental analysis of AgNCs@GO.

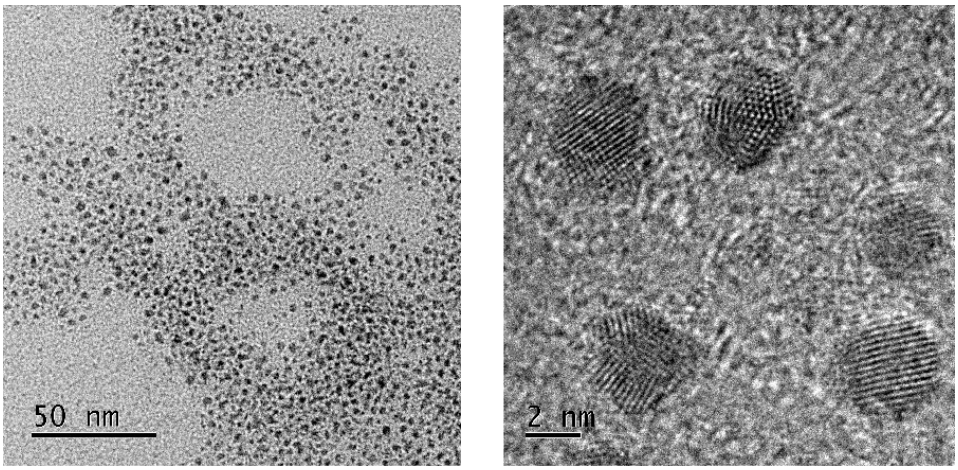

Figure S9. TEM images of AgNCs.

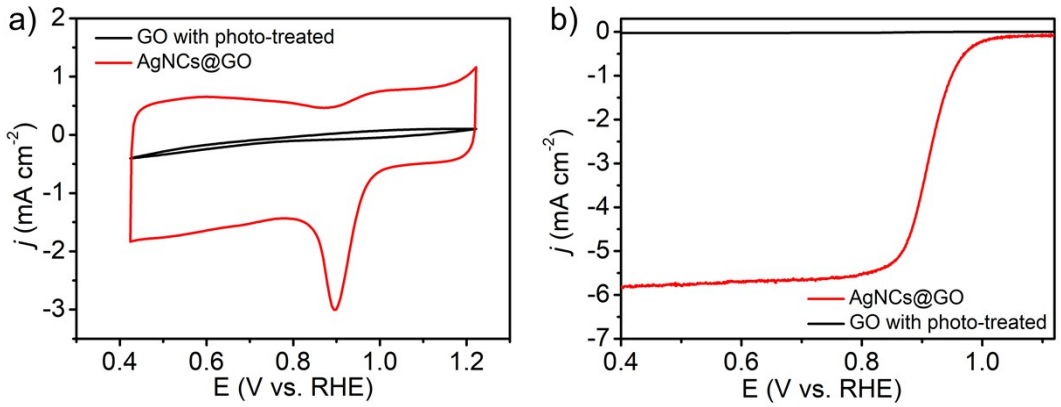

Figure S10. a), b). CV and LSV curves of GO with photo-treated and AgNCs@GO in O_2 saturated 0.1 M KOH.

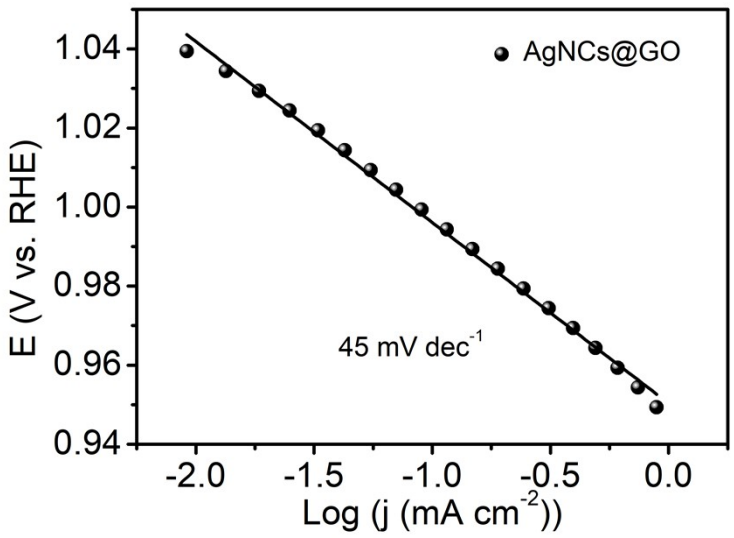

Figure S11. Tafel plots of AgNCs@GO.

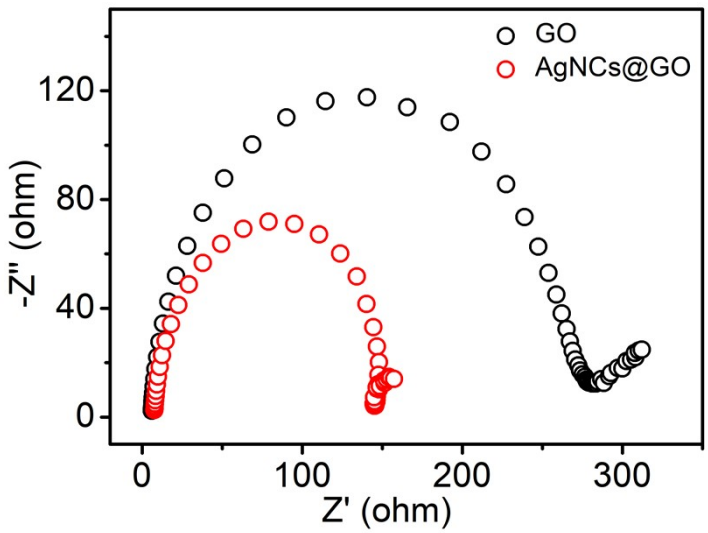

Figure S12. EIS plots of GO and AgNCs@GO.

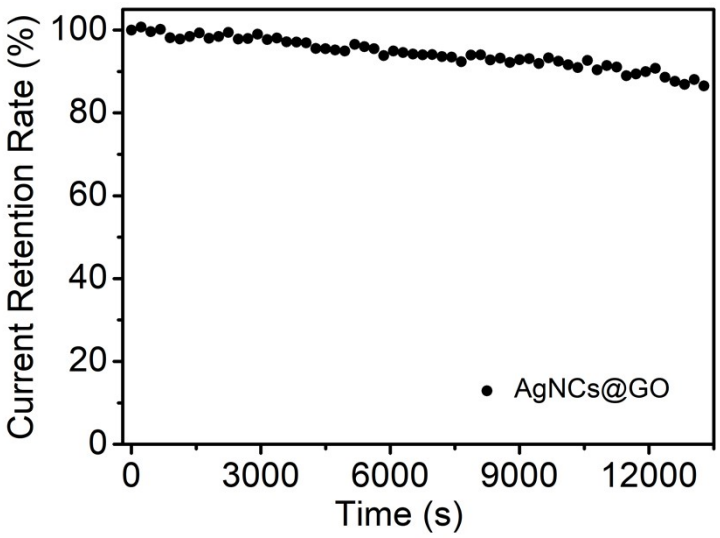

Figure S13. ORR chronoamperometric stability of AgNCs@GO in air-saturated 0.1 M KOH. Applied potential: 0.9 V vs. RHE.

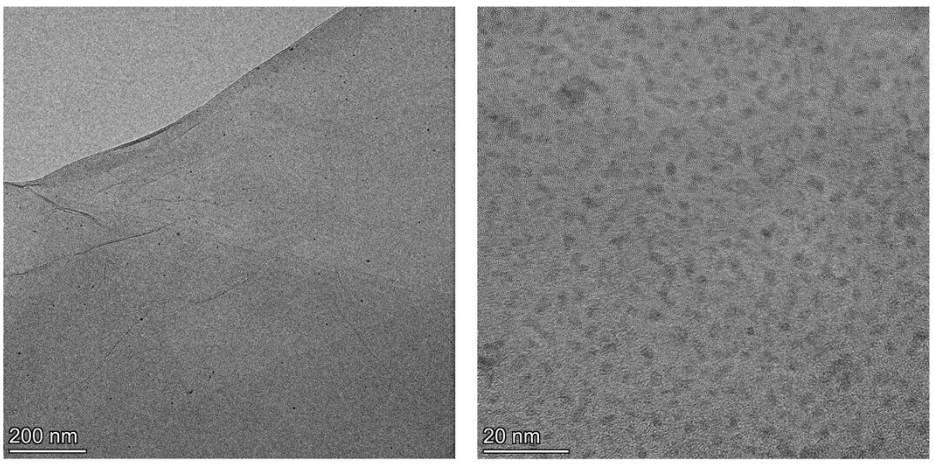

Figure S14. TEM images of AgNCs@GO after ORR.

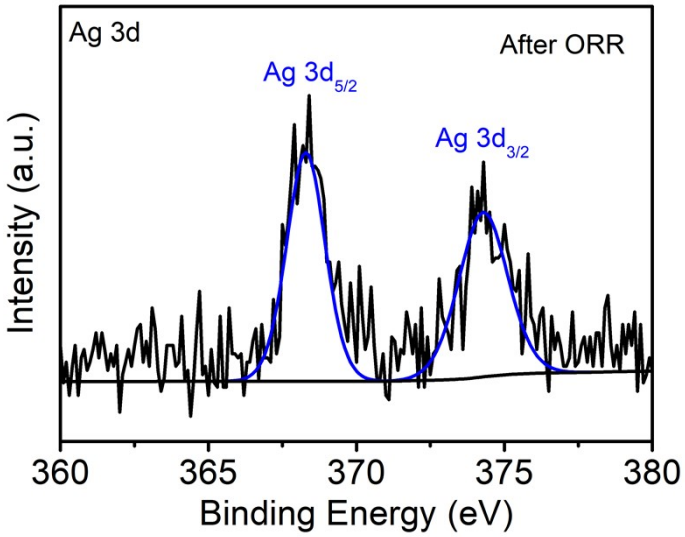

Figure S15. High resolution XPS spectra of Ag 3d of AgNCs@GO after ORR.

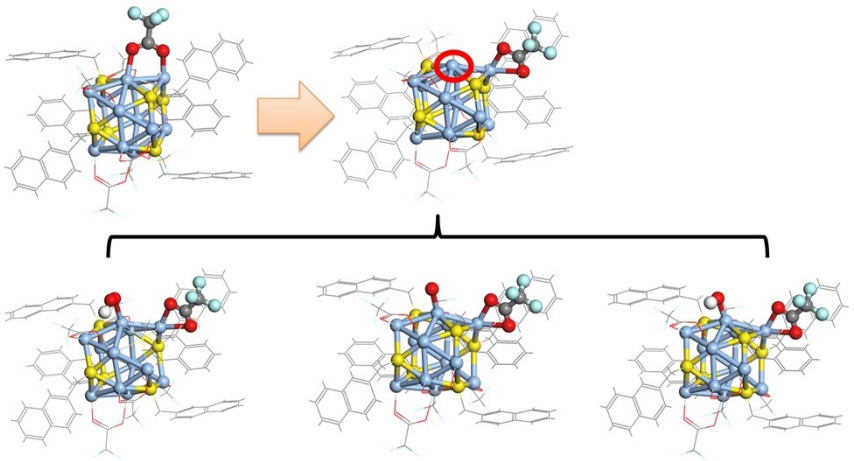

Figure S16. The deformation process of A12 clusters in oxygen reduction reactions.

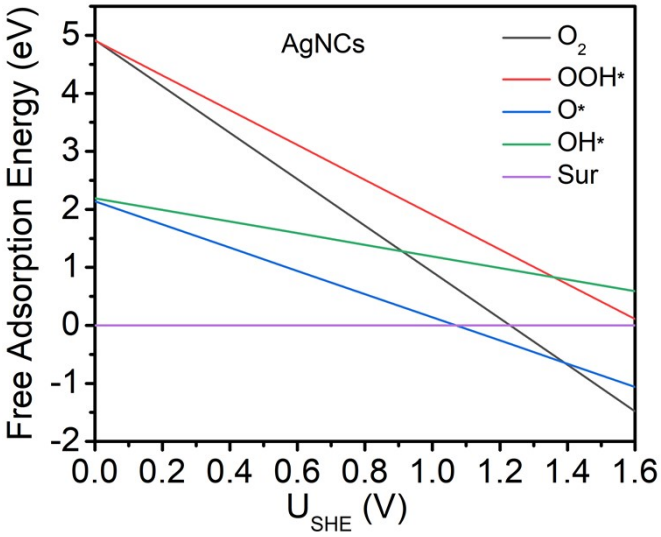

Figure S17. The free adsorption energy of intermediate on the surface of AgNCs.

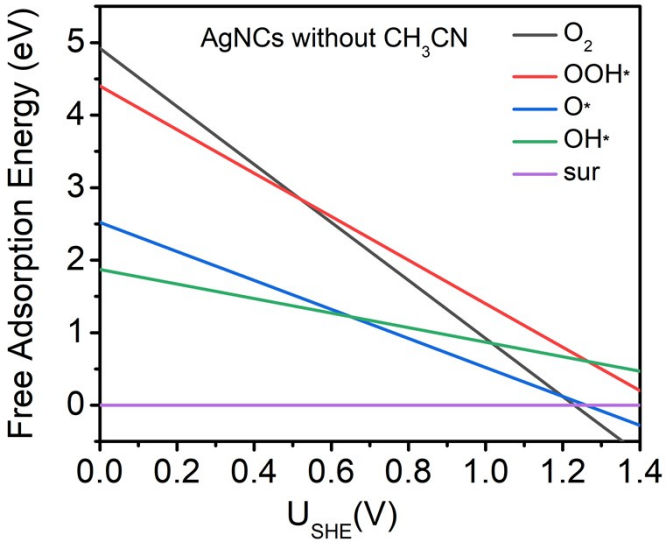

Figure S18. The free adsorption energy of intermediate on the surface of AgNCs without CH_3CN.

Table S1. Comparison of ORR performance of AgNCs@GO in this work with other reported catalysts. All catalysts were tested with a rotation speed of 1600 rpm.

Sample	Electrolyte	Onset potential (V)	Half-wave potential (V)	Tafel Slope ($mV\ dec^{-1}$)	Ref
Pd_8	0.1 M KOH	1.0	0.9	65	6
Pd_2	0.1 M KOH	0.88	0.75	80.4	6
$Ag_{22}(dppf)_3(SAdm)_{12}/C$	0.1 M KOH	0.82	0.63	-	7
$Au_1Ag_{21}(dppf)_3(SAdm)_{12}/C$	0.1 M KOH	0.86	0.66	-	7
$Fe–N–C/Pd_{NC}$	0.1 M $HClO_4$	0.97	0.87	51.1	8
Sn_xNC	0.1 M $HClO_4$	0.92	0.79	123	9
FeNCs	0.1 M KOH	1.0	0.88	-	10
AgNCs@GO	0.1 M KOH	1.0	0.91	45	This work

Table S2. CF_3CO_2 deformation.

AtomType	X	Y	Z
H	17.41363654	10.73075954	24.32768046
H	15.44726814	11.046732	22.84929513
H	19.76394785	9.37947023	20.97287178
H	19.56300709	9.87986104	23.3929646
H	16.77019358	9.59064373	17.2318983
H	14.42166504	10.9175285	20.59874653
H	18.74496802	9.2919429	18.71178925
H	18.62357752	15.04566469	6.08842492
H	17.84330682	13.37440953	7.74792015
H	21.0259367	16.97660801	9.10748094
H	20.21148248	16.84448986	6.76743596
H	17.82879051	12.51382335	10.07378965
H	20.25499454	14.42670469	13.08592468
H	21.06970659	16.06703308	11.41290038
H	11.96743765	18.08799248	5.86538404
H	13.92470615	18.1682994	7.3893629
H	9.33980655	19.11933538	9.12899136
H	9.67756769	18.55455547	6.73593878
H	12.23722025	19.58553142	12.91712433
H	14.84801603	18.46116414	9.66983109
H	10.28220748	19.53202692	11.38433128
H	13.02913925	10.58449758	5.68810477
H	12.02175298	12.22739868	7.25115895
H	13.72894003	7.85390287	8.95467638
H	13.8880364	8.4030229	6.53948396
H	12.00189255	10.11247345	12.81111001
H	11.39230787	12.87866912	9.55764859

H	13.02787816	8.4750825	11.25252038
H	10.30712508	14.24028877	24.3217206
H	11.13124541	15.94978506	22.72460997
H	8.19413515	12.23292933	21.14052951
H	8.83834599	12.38602146	23.53253424
H	9.13069655	14.83905711	17.23220944
H	11.27883147	16.81926991	20.40918588
H	8.29576066	13.13645141	18.8318485
H	16.03302911	18.99256855	24.59142923
H	17.05964504	17.3443388	23.03951382
H	15.34472786	21.70882596	21.30770444
H	15.17677126	21.16815668	23.72460365
H	17.12807223	19.43984216	17.4826616
H	17.74707771	16.71322784	20.76754152
H	16.05631652	21.06847211	19.0142852
H	18.65083411	17.38649853	17.28880226
H	18.64123	16.16308024	18.60230147
H	14.33644115	9.85083055	17.03481674
H	13.33693984	10.40508919	18.42024564
H	10.25048818	17.01778962	16.84923827
H	11.24773053	17.78547879	18.1356275
H	10.54673395	13.40482971	11.79804593
H	18.039156	11.51664748	12.32084959
H	15.78059918	18.96537086	11.87847912
H	10.6422626	12.17273269	13.10800462
H	14.70616053	19.55367746	13.20262223
H	19.0916313	12.28723881	13.55626791
O	18.25236538	13.56054615	19.31135416
O	16.43216269	13.89544838	20.62014877

O	13.57824099	19.41612603	17.70940482
O	13.07908306	19.56285032	15.48008322
O	10.72504399	11.71635692	17.49808251
O	11.19528836	11.02893386	15.36510944
O	10.32496758	16.2837501	12.17329502
O	9.76172581	15.8252083	14.34502243
O	15.60638721	10.0937293	12.59150415
O	16.04344396	9.88896381	14.83050942
O	17.99531006	17.48503285	12.07267463
O	18.40700914	17.81277347	14.28802192
Ag	17.48240547	14.55183657	15.49600481
Ag	14.71610853	17.5184435	17.61025249
Ag	13.30983475	17.28702999	15.10958611
Ag	11.92825052	13.59446739	17.49060273
Ag	13.07931831	12.3906163	15.14810979
Ag	16.36377392	13.35906682	18.07549238
Ag	11.82502409	14.90008572	14.91829544
Ag	14.54164473	12.02114859	12.74224519
Ag	15.91373553	12.18190286	15.40564477
Ag	16.87553088	15.60273359	12.6914674
Ag	16.12910558	17.00791574	15.11480033
Ag	12.50474337	16.29540694	12.50277578
S	16.63377735	16.02166183	17.31706738
S	12.43974752	15.98219226	17.08253681
S	14.34264474	12.26665236	17.2934854
S	12.64577959	13.53293812	12.95981436
S	16.88708426	13.30442816	13.42327505
S	14.73950341	17.1360523	13.04746806
F	17.95882569	13.99179571	22.82303094

F	19.54830661	12.96201625	21.71607971
F	19.30180955	15.13728689	21.51886761
F	13.61807144	22.16206613	17.63985872
F	12.54046293	22.14656501	15.73224663
F	11.52804957	21.47272054	17.56391644
F	8.49133987	10.2345339	17.44406104
F	8.90126044	9.63684681	15.37683963
F	10.0501649	8.74004465	17.02468872
F	7.98926583	17.66938287	12.03905403
F	7.32391111	16.80284135	13.93935889
F	7.4672063	15.53365068	12.15133488
F	15.38165422	7.38145631	12.56658017
F	16.28687091	7.25340425	14.5582053
F	17.51110278	7.86663122	12.8361842
F	20.01131006	19.1919675	11.49814456
F	20.31356607	19.59692177	13.62944126
F	18.54984201	20.41620444	12.59887486
C	17.50030561	17.95626029	19.03645813
C	18.05582176	16.94119629	18.09444665
C	16.30795235	19.8396661	20.78298032
C	17.65969357	13.77340789	20.42381465
C	17.0151994	19.20320144	18.5437256
C	17.38273352	17.66601112	20.3825283
C	16.7997015	18.58780577	21.2850058
C	18.6187959	13.94807676	21.63576364
C	16.43449555	20.11809925	19.39632296
C	16.11207929	19.21760066	23.52624535
C	16.68408921	18.30113645	22.66946375
C	15.72144062	20.7575787	21.69068992

C	15.62797265	20.45351436	23.03358972
C	10.27839467	15.93277503	18.72609972
C	10.90336905	16.83323207	17.71132171
C	9.28831981	14.00849456	20.55396258
C	13.17870724	19.99622182	16.65793418
C	9.4211564	14.88103265	18.28567743
C	10.61386641	16.0218063	20.06559669
C	10.13434644	15.07705527	21.00857734
C	12.71613683	21.46760477	16.89118802
C	8.93965339	13.94704265	19.17873859
C	10.02641238	14.18577301	23.26847434
C	10.48502809	15.13823986	22.38237082
C	8.83282618	13.04660421	21.49152338
C	9.19428406	13.13258671	22.82025039
C	15.46315103	10.26828664	18.83163213
C	14.30787184	10.50207346	17.91604757
C	17.71303606	9.90734691	20.51451086
C	10.57805291	11.00571651	16.46172344
C	16.70207066	9.81408948	18.29956233
C	15.3636051	10.54666846	20.18539488
C	16.46740018	10.37352281	21.05661213
C	9.48170368	9.89971297	16.57613039
C	17.79427145	9.64167608	19.12187397
C	17.48182383	10.48763978	23.2650572
C	16.38652599	10.66313057	22.44420826
C	18.81608548	9.72962452	21.38720333
C	18.70217006	10.00832105	22.73406922
C	11.65242933	11.61433635	11.27718329
C	11.16956707	12.62790099	12.26043283

C	12.78177661	9.72511999	9.49582815
C	9.53832473	16.18893209	13.16282093
C	12.11235586	10.3513547	11.75003439
C	11.74298085	11.91114442	9.92886632
C	12.29682954	10.98603814	9.00753289
C	8.06025232	16.56082399	12.82809913
C	12.66429034	9.43546984	10.88136255
C	12.95994083	10.35606175	6.75322204
C	12.39912019	11.27061176	7.62058496
C	13.35651702	8.80919312	8.57784301
C	13.44486644	9.11715202	7.23578408
C	18.97994602	13.36571508	11.67816013
C	18.40338013	12.47149596	12.72310227
C	19.90809047	15.24636853	9.77662771
C	15.93312849	9.47590288	13.64872455
C	19.90929549	14.37783766	12.05035775
C	18.54201657	13.29025935	10.36618173
C	18.98685021	14.21495551	9.38802033
C	16.27473665	7.97177821	13.40939104
C	20.36001569	15.28904587	11.12217575
C	18.97499682	15.09310389	7.12061986
C	18.53928627	14.1637398	8.0417186
C	20.333825	16.18726434	8.80525499
C	19.87766368	16.11298163	7.50546902
C	13.66803509	19.002085	11.38267189
C	14.79505987	18.86910452	12.35064625
C	11.44035524	18.97639682	9.63784217
C	18.52190974	18.07459299	13.0463013
C	12.36441793	19.3203791	11.86402469

C	13.84946887	18.70683119	10.04262596
C	12.75696503	18.69102237	9.13960844
C	19.3763416	19.32865987	12.6883623
C	11.28265096	19.30535885	11.01041704
C	11.83058938	18.33149221	6.92055612
C	12.91991392	18.37623492	7.76520341
C	10.34138907	18.91613843	8.74366521
C	10.53141217	18.59897634	7.41436779

OOH-CF_3CO_2 deformation

AtomType	X	Y	Z
H	19.52066591	16.96006515	15.04197657
H	17.41363654	10.73075954	24.32768046
H	15.44726814	11.046732	22.84929513
H	19.76394785	9.37947023	20.97287178
H	19.56300709	9.87986104	23.3929646
H	16.77019358	9.59064373	17.2318983
H	14.42166504	10.9175285	20.59874653
H	18.74496802	9.2919429	18.71178925
H	18.62357752	15.04566469	6.08842492
H	17.84330682	13.37440953	7.74792015
H	21.0259367	16.97660801	9.10748094
H	20.21148248	16.84448986	6.76743596
H	17.82879051	12.51382335	10.07378965
H	20.25499454	14.42670469	13.08592468
H	21.06970659	16.06703308	11.41290038
H	11.96743765	18.08799248	5.86538404
H	13.92470615	18.1682994	7.3893629
H	9.33980655	19.11933538	9.12899136
H	9.67756769	18.55455547	6.73593878

H	12.23722025	19.58553142	12.91712433
H	14.84801603	18.46116414	9.66983109
H	10.28220748	19.53202692	11.38433128
H	13.02913925	10.58449758	5.68810477
H	12.02175298	12.22739868	7.25115895
H	13.72894003	7.85390287	8.95467638
H	13.8880364	8.4030229	6.53948396
H	12.00189255	10.11247345	12.81111001
H	11.39230787	12.87866912	9.55764859
H	13.02787816	8.4750825	11.25252038
H	10.30712508	14.24028877	24.3217206
H	11.13124541	15.94978506	22.72460997
H	8.19413515	12.23292933	21.14052951
H	8.83834599	12.38602146	23.53253424
H	9.13069655	14.83905711	17.23220944
H	11.27883147	16.81926991	20.40918588
H	8.29576066	13.13645141	18.8318485
H	16.03302911	18.99256855	24.59142923
H	17.05964504	17.3443388	23.03951382
H	15.34472786	21.70882596	21.30770444
H	15.17677126	21.16815668	23.72460365
H	17.12807223	19.43984216	17.4826616
H	17.74707771	16.71322784	20.76754152
H	16.05631652	21.06847211	19.0142852
H	18.65083411	17.38649853	17.28880226
H	18.64123	16.16308024	18.60230147
H	14.33644115	9.85083055	17.03481674
H	13.33693984	10.40508919	18.42024564
H	10.25048818	17.01778962	16.84923827

H	11.24773053	17.78547879	18.1356275
H	10.54673395	13.40482971	11.79804593
H	18.039156	11.51664748	12.32084959
H	15.78059918	18.96537086	11.87847912
H	10.6422626	12.17273269	13.10800462
H	14.70616053	19.55367746	13.20262223
H	19.0916313	12.28723881	13.55626791
O	19.79810307	15.1183066	15.48863947
O	20.22592953	16.40341015	15.53833723
O	18.25236538	13.56054615	19.31135416
O	16.43216269	13.89544838	20.62014877
O	13.57824099	19.41612603	17.70940482
O	13.07908306	19.56285032	15.48008322
O	10.72504399	11.71635692	17.49808251
O	11.19528836	11.02893386	15.36510944
O	10.32496758	16.2837501	12.17329502
O	9.76172581	15.8252083	14.34502243
O	15.60638721	10.0937293	12.59150415
O	16.04344396	9.88896381	14.83050942
O	17.99531006	17.48503285	12.07267463
O	18.40700914	17.81277347	14.28802192
Ag	17.48240547	14.55183657	15.49600481
Ag	14.71610853	17.5184435	17.61025249
Ag	13.30983475	17.28702999	15.10958611
Ag	11.92825052	13.59446739	17.49060273
Ag	13.07931831	12.3906163	15.14810979
Ag	16.36377392	13.35906682	18.07549238
Ag	11.82502409	14.90008572	14.91829544
Ag	14.54164473	12.02114859	12.74224519

Ag	15.91373553	12.18190286	15.40564477
Ag	16.87553088	15.60273359	12.6914674
Ag	16.12910558	17.00791574	15.11480033
Ag	12.50474337	16.29540694	12.50277578
S	16.63377735	16.02166183	17.31706738
S	12.43974752	15.98219226	17.08253681
S	14.34264474	12.26665236	17.2934854
S	12.64577959	13.53293812	12.95981436
S	16.88708426	13.30442816	13.42327505
S	14.73950341	17.1360523	13.04746806
F	17.95882569	13.99179571	22.82303094
F	19.54830661	12.96201625	21.71607971
F	19.30180955	15.13728689	21.51886761
F	13.61807144	22.16206613	17.63985872
F	12.54046293	22.14656501	15.73224663
F	11.52804957	21.47272054	17.56391644
F	8.49133987	10.2345339	17.44406104
F	8.90126044	9.63684681	15.37683963
F	10.0501649	8.74004465	17.02468872
F	7.98926583	17.66938287	12.03905403
F	7.32391111	16.80284135	13.93935889
F	7.4672063	15.53365068	12.15133488
F	15.38165422	7.38145631	12.56658017
F	16.28687091	7.25340425	14.5582053
F	17.51110278	7.86663122	12.8361842
F	20.01131006	19.1919675	11.49814456
F	20.31356607	19.59692177	13.62944126
F	18.54984201	20.41620444	12.59887486
C	17.50030561	17.95626029	19.03645813

C	18.05582176	16.94119629	18.09444665
C	16.30795235	19.8396661	20.78298032
C	17.65969357	13.77340789	20.42381465
C	17.0151994	19.20320144	18.5437256
C	17.38273352	17.66601112	20.3825283
C	16.7997015	18.58780577	21.2850058
C	18.6187959	13.94807676	21.63576364
C	16.43449555	20.11809925	19.39632296
C	16.11207929	19.21760066	23.52624535
C	16.68408921	18.30113645	22.66946375
C	15.72144062	20.7575787	21.69068992
C	15.62797265	20.45351436	23.03358972
C	10.27839467	15.93277503	18.72609972
C	10.90336905	16.83323207	17.71132171
C	9.28831981	14.00849456	20.55396258
C	13.17870724	19.99622182	16.65793418
C	9.4211564	14.88103265	18.28567743
C	10.61386641	16.0218063	20.06559669
C	10.13434644	15.07705527	21.00857734
C	12.71613683	21.46760477	16.89118802
C	8.93965339	13.94704265	19.17873859
C	10.02641238	14.18577301	23.26847434
C	10.48502809	15.13823986	22.38237082
C	8.83282618	13.04660421	21.49152338
C	9.19428406	13.13258671	22.82025039
C	15.46315103	10.26828664	18.83163213
C	14.30787184	10.50207346	17.91604757
C	17.71303606	9.90734691	20.51451086
C	10.57805291	11.00571651	16.46172344

C	16.70207066	9.81408948	18.29956233
C	15.3636051	10.54666846	20.18539488
C	16.46740018	10.37352281	21.05661213
C	9.48170368	9.89971297	16.57613039
C	17.79427145	9.64167608	19.12187397
C	17.48182383	10.48763978	23.2650572
C	16.38652599	10.66313057	22.44420826
C	18.81608548	9.72962452	21.38720333
C	18.70217006	10.00832105	22.73406922
C	11.65242933	11.61433635	11.27718329
C	11.16956707	12.62790099	12.26043283
C	12.78177661	9.72511999	9.49582815
C	9.53832473	16.18893209	13.16282093
C	12.11235586	10.3513547	11.75003439
C	11.74298085	11.91114442	9.92886632
C	12.29682954	10.98603814	9.00753289
C	8.06025232	16.56082399	12.82809913
C	12.66429034	9.43546984	10.88136255
C	12.95994083	10.35606175	6.75322204
C	12.39912019	11.27061176	7.62058496
C	13.35651702	8.80919312	8.57784301
C	13.44486644	9.11715202	7.23578408
C	18.97994602	13.36571508	11.67816013
C	18.40338013	12.47149596	12.72310227
C	19.90809047	15.24636853	9.77662771
C	15.93312849	9.47590288	13.64872455
C	19.90929549	14.37783766	12.05035775
C	18.54201657	13.29025935	10.36618173
C	18.98685021	14.21495551	9.38802033

C	16.27473665	7.97177821	13.40939104
C	20.36001569	15.28904587	11.12217575
C	18.97499682	15.09310389	7.12061986
C	18.53928627	14.1637398	8.0417186
C	20.333825	16.18726434	8.80525499
C	19.87766368	16.11298163	7.50546902
C	13.66803509	19.002085	11.38267189
C	14.79505987	18.86910452	12.35064625
C	11.44035524	18.97639682	9.63784217
C	18.52190974	18.07459299	13.0463013
C	12.36441793	19.3203791	11.86402469
C	13.84946887	18.70683119	10.04262596
C	12.75696503	18.69102237	9.13960844
C	19.3763416	19.32865987	12.6883623
C	11.28265096	19.30535885	11.01041704
C	11.83058938	18.33149221	6.92055612
C	12.91991392	18.37623492	7.76520341
C	10.34138907	18.91613843	8.74366521
C	10.53141217	18.59897634	7.41436779

O-CF_3CO_2 deformation

AtomType	X	Y	Z
H	17.41363654	10.73075954	24.32768046
H	15.44726814	11.046732	22.84929513
H	19.76394785	9.37947023	20.97287178
H	19.56300709	9.87986104	23.3929646
H	16.77019358	9.59064373	17.2318983
H	14.42166504	10.9175285	20.59874653
H	18.74496802	9.2919429	18.71178925
H	18.62357752	15.04566469	6.08842492

H	17.84330682	13.37440953	7.74792015
H	21.0259367	16.97660801	9.10748094
H	20.21148248	16.84448986	6.76743596
H	17.82879051	12.51382335	10.07378965
H	20.25499454	14.42670469	13.08592468
H	21.06970659	16.06703308	11.41290038
H	11.96743765	18.08799248	5.86538404
H	13.92470615	18.1682994	7.3893629
H	9.33980655	19.11933538	9.12899136
H	9.67756769	18.55455547	6.73593878
H	12.23722025	19.58553142	12.91712433
H	14.84801603	18.46116414	9.66983109
H	10.28220748	19.53202692	11.38433128
H	13.02913925	10.58449758	5.68810477
H	12.02175298	12.22739868	7.25115895
H	13.72894003	7.85390287	8.95467638
H	13.8880364	8.4030229	6.53948396
H	12.00189255	10.11247345	12.81111001
H	11.39230787	12.87866912	9.55764859
H	13.02787816	8.4750825	11.25252038
H	10.30712508	14.24028877	24.3217206
H	11.13124541	15.94978506	22.72460997
H	8.19413515	12.23292933	21.14052951
H	8.83834599	12.38602146	23.53253424
H	9.13069655	14.83905711	17.23220944
H	11.27883147	16.81926991	20.40918588
H	8.29576066	13.13645141	18.8318485
H	16.03302911	18.99256855	24.59142923
H	17.05964504	17.3443388	23.03951382

H	15.34472786	21.70882596	21.30770444
H	15.17677126	21.16815668	23.72460365
H	17.12807223	19.43984216	17.4826616
H	17.74707771	16.71322784	20.76754152
H	16.05631652	21.06847211	19.0142852
H	18.65083411	17.38649853	17.28880226
H	18.64123	16.16308024	18.60230147
H	14.33644115	9.85083055	17.03481674
H	13.33693984	10.40508919	18.42024564
H	10.25048818	17.01778962	16.84923827
H	11.24773053	17.78547879	18.1356275
H	10.54673395	13.40482971	11.79804593
H	18.039156	11.51664748	12.32084959
H	15.78059918	18.96537086	11.87847912
H	10.6422626	12.17273269	13.10800462
H	14.70616053	19.55367746	13.20262223
H	19.0916313	12.28723881	13.55626791
O	19.52444275	14.5230547	15.29504656
O	18.25236538	13.56054615	19.31135416
O	16.43216269	13.89544838	20.62014877
O	13.57824099	19.41612603	17.70940482
O	13.07908306	19.56285032	15.48008322
O	10.72504399	11.71635692	17.49808251
O	11.19528836	11.02893386	15.36510944
O	10.32496758	16.2837501	12.17329502
O	9.76172581	15.8252083	14.34502243
O	15.60638721	10.0937293	12.59150415
O	16.04344396	9.88896381	14.83050942
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Ag	14.71610853	17.5184435	17.61025249
Ag	13.30983475	17.28702999	15.10958611
Ag	11.92825052	13.59446739	17.49060273
Ag	13.07931831	12.3906163	15.14810979
Ag	16.36377392	13.35906682	18.07549238
Ag	11.82502409	14.90008572	14.91829544
Ag	14.54164473	12.02114859	12.74224519
Ag	15.91373553	12.18190286	15.40564477
Ag	16.87553088	15.60273359	12.6914674
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Ag	12.50474337	16.29540694	12.50277578
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S	14.34264474	12.26665236	17.2934854
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C	12.91991392	18.37623492	7.76520341
C	10.34138907	18.91613843	8.74366521
C	10.53141217	18.59897634	7.41436779
$OH\text{-}CF_3CO_2$ deformation			

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H	16.77019358	9.59064373	17.2318983
H	14.42166504	10.9175285	20.59874653
H	18.74496802	9.2919429	18.71178925
H	18.62357752	15.04566469	6.08842492
H	17.84330682	13.37440953	7.74792015
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H	20.21148248	16.84448986	6.76743596
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F	19.54830661	12.96201625	21.71607971
F	19.30180955	15.13728689	21.51886761
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F	7.32391111	16.80284135	13.93935889
F	7.4672063	15.53365068	12.15133488
F	15.38165422	7.38145631	12.56658017
F	16.28687091	7.25340425	14.5582053
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F	20.01131006	19.1919675	11.49814456
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C	17.65969357	13.77340789	20.42381465
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C	17.38273352	17.66601112	20.3825283
C	16.7997015	18.58780577	21.2850058
C	18.6187959	13.94807676	21.63576364
C	16.43449555	20.11809925	19.39632296
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C	16.68408921	18.30113645	22.66946375

C	15.72144062	20.7575787	21.69068992
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C	10.90336905	16.83323207	17.71132171
C	9.28831981	14.00849456	20.55396258
C	13.17870724	19.99622182	16.65793418
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