# Supporting information for the paper:

## Detection of $[Au_{25}(PET)_{18}(O_2)_n]^-$ (n=1,2,3) Species by Mass Spectrometry

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## Table of Contents

**Supporting information 1**

## Characterization of $[Au_{25}(PET)_{18}]^-$:

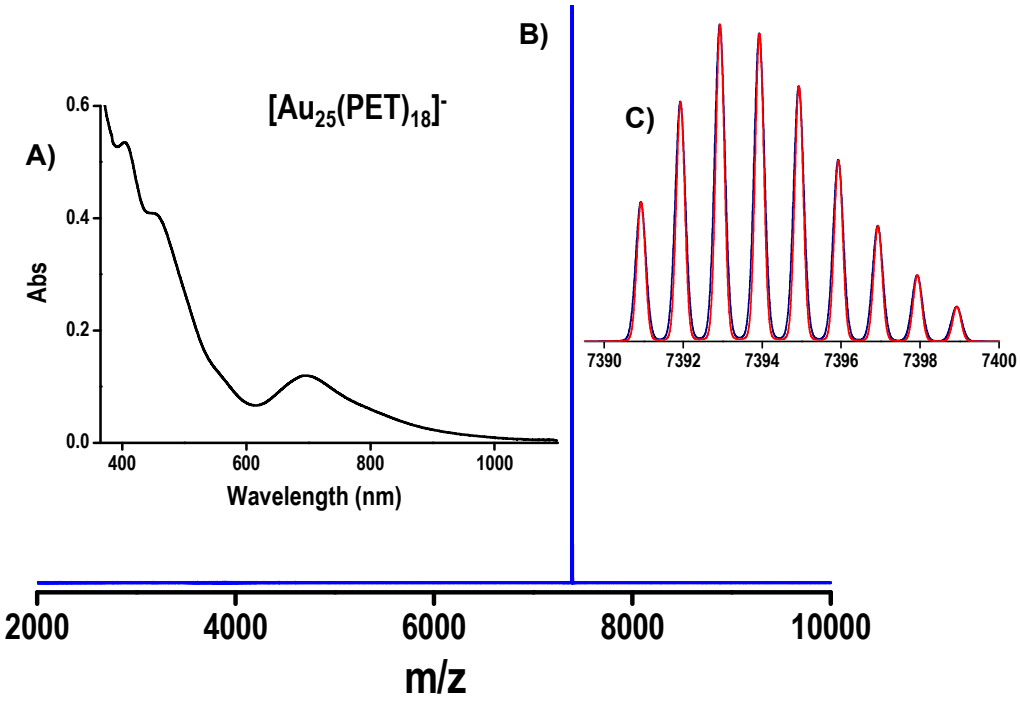


**Figure S1.** A) UV/Vis absorption spectrum and B) ESI MS of $[Au_{25}(PET)_{18}]^-$. C) Experimental (blue trace) and simulated (red trace) mass spectra of $[Au_{25}(PET)_{18}]^-$.

**Supporting information 2**

**Stability of $[Au_{25}(PET)_{18}]^-$ kept in continuous flow of $O_2$ in DCM:**

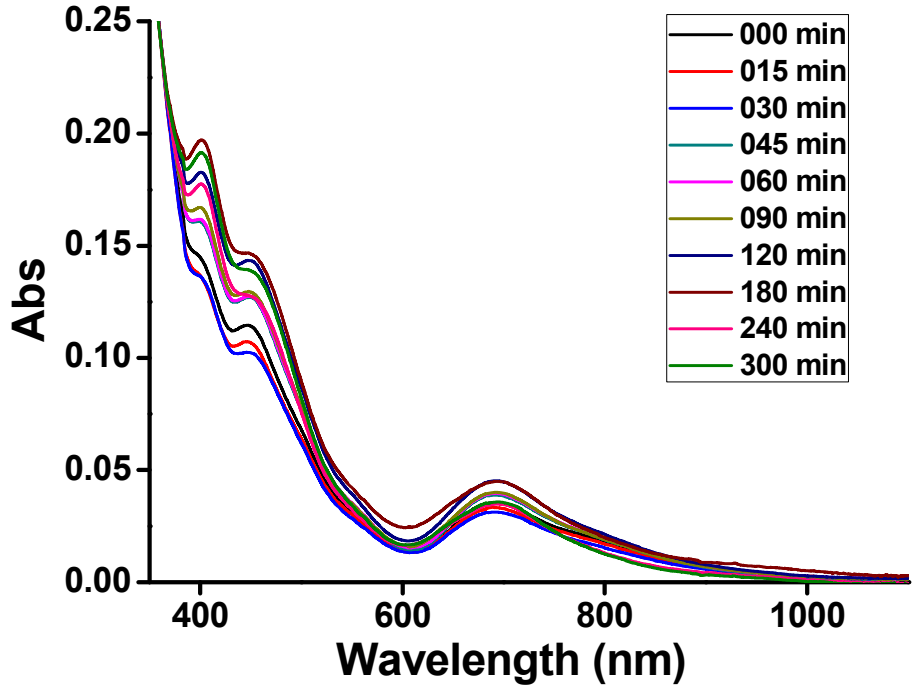


**Figure S2.** Time – dependent UV/Vis absorption spectra of $[Au_{25}(PET)_{18}]^-$ kept under continuous flow of $O_2$ in DCM.

**Supporting Information 3**

## Comparison of UV/Vis spectra of air oxidized and $O_2$ treated $Au_{25}(PET)_{18}$:

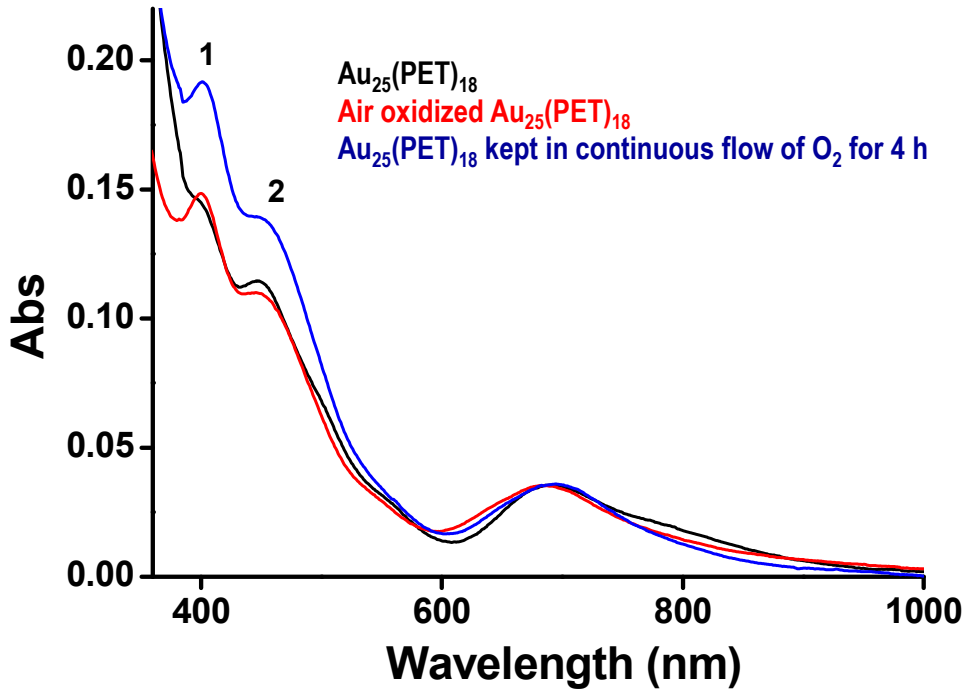


**Figure S3.** Comparison of UV/Vis absorption spectra for $[Au_{25}(PET)_{18}]^-$ (black trace), air oxidized nanocluater, i.e. $[Au_{25}(PET)_{18}]^0$ (red trace) and the same under continuous flow of $O_2$ for 4 h. The spectra are normalized at 680 nm. Peaks 1 and 2 are 400 and 450 nm absorption features of the cluster.

## Supporting Information 4

## Experimental and simulated mass spectra for $[Au_{25}(PET)_{18}(O_2)_2]^-$ and $[Au_{25}(PET)_{18}(O_2)_3]^-$:

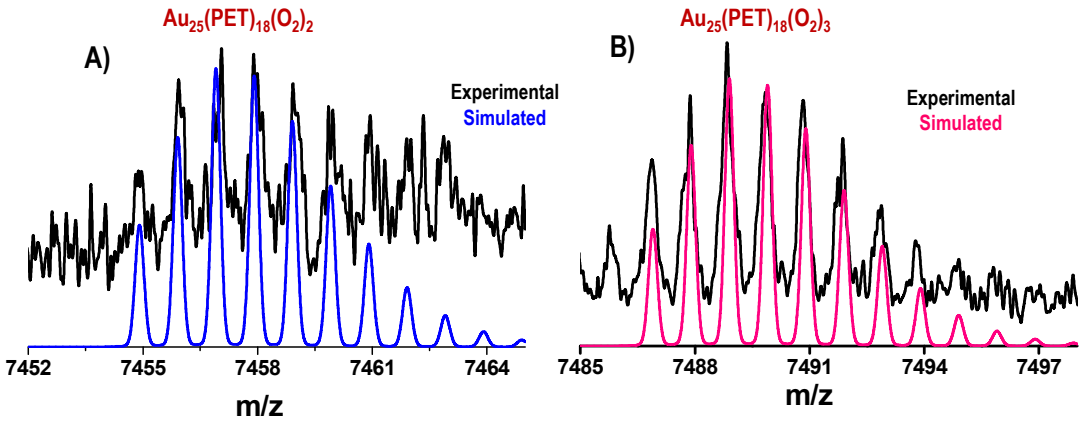


**Figure S4.** A) Experimental and simulated mass spectra of $[Au_{25}(PET)_{18}(O_2)_2]^-$and B) $[Au_{25}(PET)_{18}(O_2)_3]^-$.

## Supporting Information 5

## Stability of $[Au_{25}(PET)_{18}]^-$ in continuous flow of $O_2$ in toluene and THF:

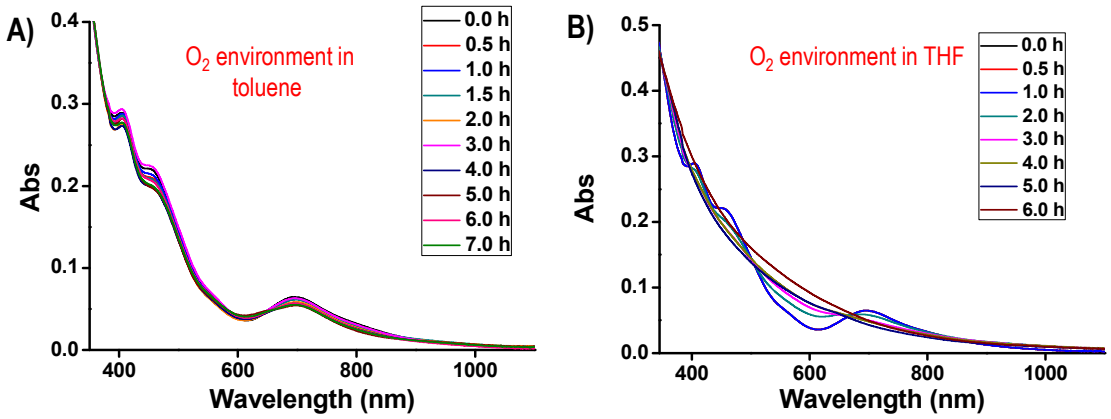


**Figure S5.** A) Time – dependent UV/Vis absorption spectra of $[Au_{25}(PET)_{18}]^-$ kept under continuous flow of $O_2$ in toluene and B) in THF.

## Supporting Information 6

## Time-dependent ESI MS of $[Au_{25}(PET)_{18}]^-$ kept in continuous flow of $O_2$ in THF:

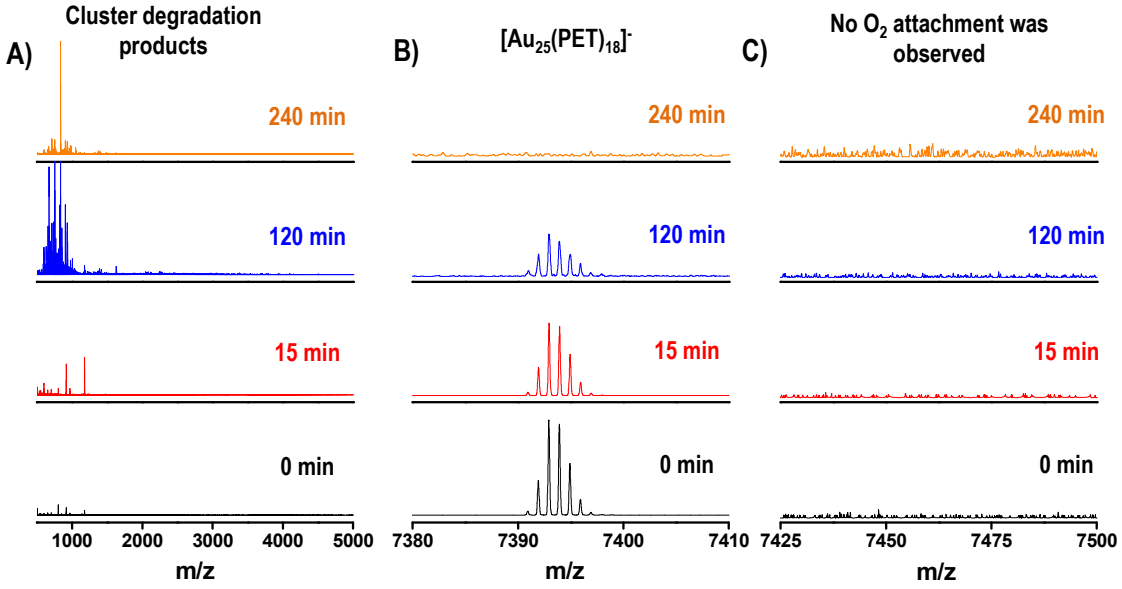


**Figure S6.** Time-dependent ESI MS upon exposure of $[Au_{25}(PET)_{18}]^-$ to a continuous flow of $O_2$ in THF. Spectra in different mass range are presented in A), B) and C).

## Supporting Information 7

## Stability of $[Au_{25}(PET)_{18}]^-$ in presence of various gases:

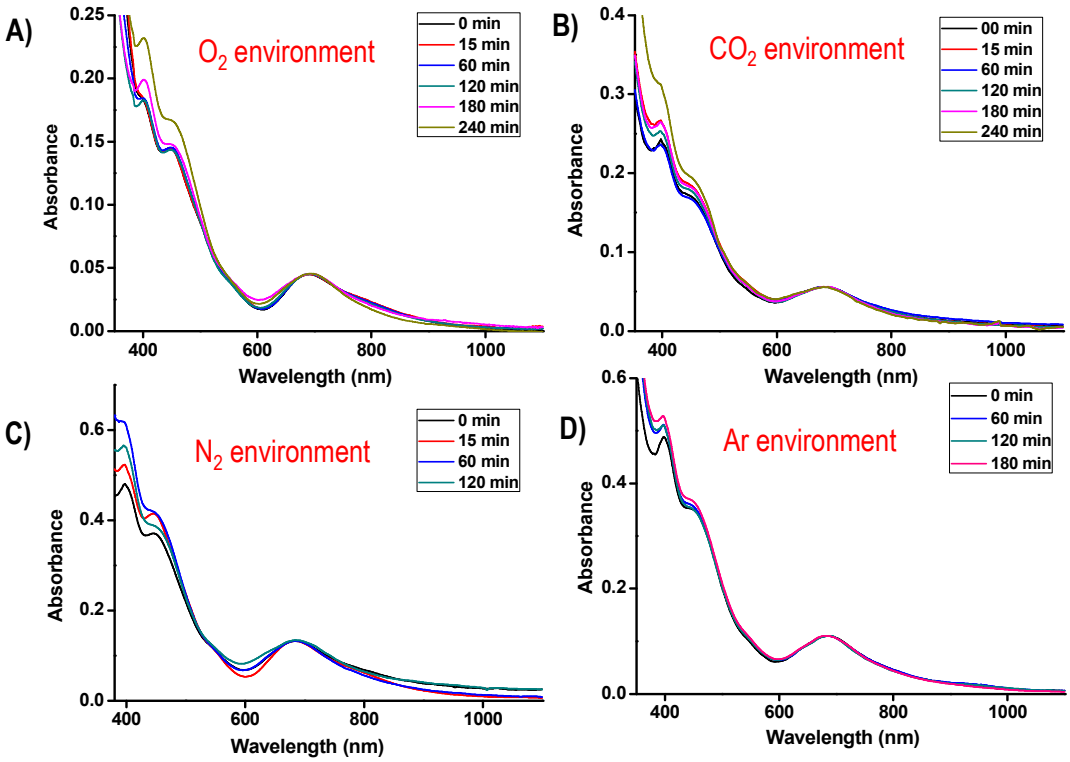


**Figure S7.** A) Time-dependent UV/Vis absorption spectra of $[Au_{25}(PET)_{18}]^-$ kept in $O_2$ environment, B) in $CO_2$ environment, C) in $N_2$ environment, and D) in Ar environment.

## Supporting Information 8

## ESI MS of $[Au_{25}(PET)_{18}]^-$ in presence of various gases:

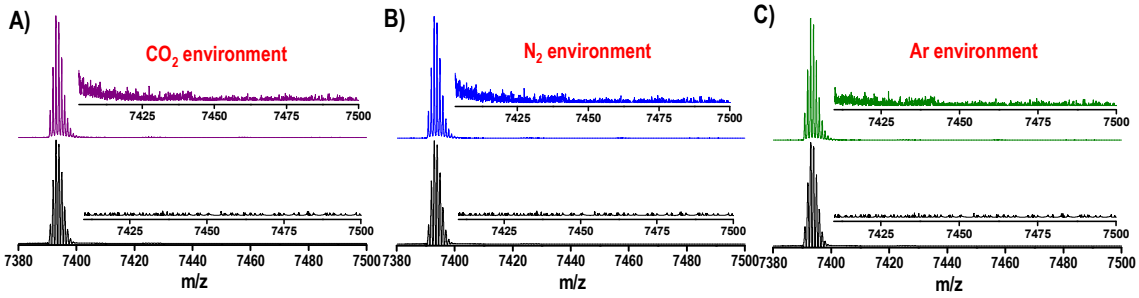


**Figure S8.** A) ESI MS of $[Au_{25}(PET)_{18}]^-$ before and after keeping in $CO_2$ environment. B) ESI MS of $[Au_{25}(PET)_{18}]^-$ before and after keeping in $N_2$ environment. C) ESI MS of $[Au_{25}(PET)_{18}]^-$ before and after keeping in Ar environment. The intensities of the parent clusters are normalised. We did not observe the adduct species in these cases.

## Supporting Information 9

## Structures of higher energy isomers of $[Au_{25}(PET)_{18}(O_2)]^-$:

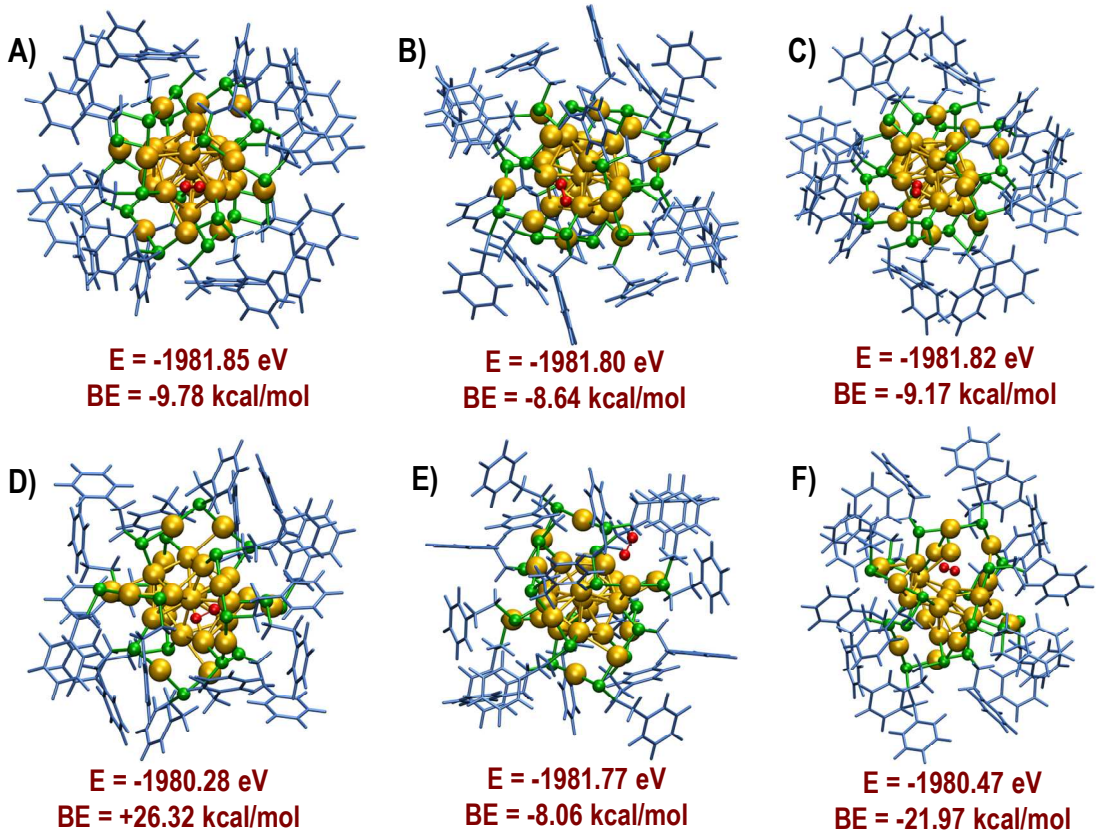


**Figure S9.** DFT optimized structures of certain higher energy isomers of $[Au_{25}(PET)_{18}(O_2)]^-$ species along with their energies and binding energies. Color codes: Golden yellow – Au, Green – S, Red – O and Blue stick models represent PET ligands.

## Supporting Information 10

## Comparison of bonding parameters of $[Au_{25}(PET)_{18}(O_2)]^-$ obtained using PBE functional and vdW-DF2 functional:

**Table S1.** Bonding parameters of $[Au_{25}(PET)_{18}(O_2)]^-$ obtained using PBE functional (without dispersion corrections) and vdW-DF2 functional (with dispersion corrections).

| Bond | Bond distance (Å) using PBE functional | Bond distance (Å) vdW-DF2 functional |
|---|---|---|
| O – O | 1.27 | 1.30 |
| Au – O (core) | 3.57 | 3.37 |
| Au – O (staple) | 3.33 | 3.38 |
| Au – Au | 2.87 | 2.97 |
| Au – S (core) | 2.44 | 2.54 |
| Au – S (staple) | 2.37 | 2.43 |

## Supporting Information 11

## Binding energy of $O_2$ on various surfaces of Au and bare clusters of Au from literature:

**Table S2.** Binding energy of $O_2$ on various surfaces of Au and bare clusters of Au, obtained from literature.

| SI. No. | Experimental/theoretical | Au surface/cluster | Binding energy (kcal/mol) | Reference* |
|---|---|---|---|---|
| 1 | Experimental (TPD)/atomic oxygen[±] | Au (1 1 1) | -30 to -32 depending on coverage | 1 |
| 2 | Experimental (TPD)/atomic oxygen[±] | Au (2 1 1) step site/terrace site | -34/-33 | 2 |
| 3 | Theoretical | 10% stretched Au (1 1 1) | -1.9 | 3 |
| 4 | Theoretical | Unstretched/10% stretched Au (2 1 1) | -3.5/-6 | 3 |
| 5 | Theoretical | $Au_{55}$ cluster | -6.9/-13.1 depending on sites | 4[ǂ] |
| 6 | Theoretical | $Au_{25+}$,$Au_{25}^{0}$,$Au_{25}^{-}$ | -13.4, -11.8, -31.6 | 5 |

*References are given at the end. [±]TPD gives the dissociation energy which is equal in quantity and opposite in sign to binding energy. To avoid confusion, the TPD-derived binding energies are presented with a negative sign. [ǂ]Authors use opposite sign convention in ref. 4. We have changed the sign to keep consistency with our convention. This makes it clear that all values correspond to bound oxygen.

**Supporting Information 12**

## DFT optimized structure of $[Au_{25}(PET)_{18}(O_2)_4]^-$:

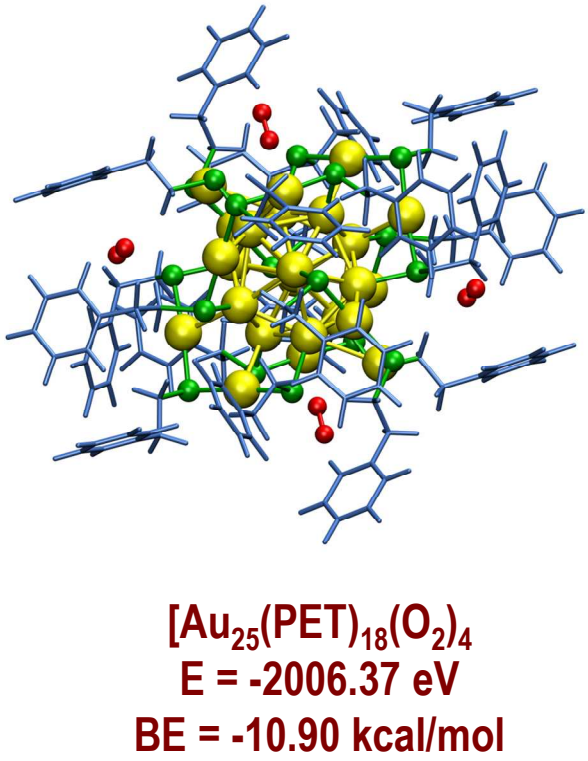


**Figure S10.** DFT optimized structures of $[Au_{25}(PET)_{18}(O_2)_4]^-$.

## Supporting information 13

## Cartesian coordinates for DFT optimized structures:

**$[Au_{25}(PET)_{18}O_2]^-$ cluster:**

Au 15.54538 18.81844 15.48189

Au 12.71730 19.70230 17.01116

Au 11.95114 16.70619 18.92236

Au 14.20123 14.51823 17.63883

Au 14.99400 16.68663 13.39163

Au 16.43253 19.68019 12.54700

Au 18.16423 20.61777 15.61596

Au 17.69625 17.83797 17.37439

Au 13.23671 16.78695 15.89420

Au 12.02516 15.84900 12.84438

Au 14.93072 14.17526 11.42720

Au 17.17697 14.57884 13.87690

Au 16.46700 13.26345 16.53739

Au 19.28962 12.35596 14.96917

Au 20.01383 15.30853 12.99681

Au 17.78139 17.54752 14.35358

Au 16.98176 15.39446 18.61580

Au 15.59946 12.44579 19.45909

Au 13.83915 11.49743 16.35521

Au 14.27931 14.24623 14.61216

Au 18.74186 15.28503 16.09649

Au 19.96997 16.24198 19.08994

Au 17.05082 17.88679 20.54336

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S 13.88870 20.58609 15.15860

S 11.44888 19.01684 18.87802

S 12.20826 14.35638 19.02059

S 17.59781 21.49437 13.50091

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S 15.09863 18.09357 11.40850

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S 12.77997 14.93888 10.80320

S 17.09443 13.30632 11.79204

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S 20.55126 13.01407 13.08814

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H 22.51625 20.35535 22.67178

C 15.18936 20.42288 19.51245

H 14.17773 20.87193 19.36353

H 15.66178 20.31148 18.50868

C 16.05481 21.29247 20.44086

H 17.07793 20.84272 20.45770

H 15.65478 21.23540 21.48086

C 16.10800 22.74012 19.98925

C 15.40691 23.74386 20.69780

H 14.84452 23.46360 21.61184

C 15.41393 25.08351 20.26134

H 14.85432 25.85035 20.83244

C 16.12609 25.44317 19.10017

H 16.13011 26.49388 18.75030

C 16.83174 24.45351 18.38535

H 17.39627 24.72260 17.47052

C 16.82516 23.11586 18.82600

H 17.39330 22.34857 18.25977

O 13.61022 14.60526 21.78745

O 14.20835 15.38035 20.97491

**$[Au_{25}(PET)_{18}(O_2)_2]^-$ cluster:**

O 10.01050 18.44753 16.74426

O 10.82431 17.68346 17.36026

O 21.92322 13.62408 15.35648

O 20.98204 14.41746 15.02667

Au 16.04034 18.80207 15.60997

Au 19.01409 19.94051 16.60694

Au 20.83595 16.87646 17.24625

Au 18.28827 14.60891 17.05865

Au 14.55592 17.53936 17.93042

Au 13.19268 20.10589 16.22405

Au 14.70275 19.72922 12.89164

Au 16.21716 16.83376 13.30956

Au 17.61914 17.41146 17.89019

Au 15.85074 17.66818 20.76058

Au 12.84998 15.76039 19.94477

Au 13.49540 14.90437 16.78868

Au 15.96862 13.14334 16.42211

Au 12.99447 11.99398 15.42569

Au 11.18405 15.08445 14.81238

Au 13.72182 17.34979 14.96314

Au 17.45039 14.42917 14.09981

Au 18.78327 11.84877 15.81759

Au 17.29715 12.24228 19.16145

Au 15.79316 15.11195 18.71963

Au 14.39171 14.53290 14.15027

Au 16.16332 14.29784 11.26599

Au 19.16378 16.19662 12.09440

Au 18.50947 17.05621 15.24542

Au 15.99909 15.97745 16.01925

S 16.88921 20.95136 16.38300

S 21.23009 19.16159 16.82085

S 20.58045 14.61062 17.85209

S 13.39890 21.23133 14.16637

S 15.97186 18.36744 11.42542

S 13.01426 19.32244 18.45011

S 18.06868 18.18185 20.15065

S 13.70411 17.19362 21.61479

S 11.79351 14.29498 18.43433

S 15.11870 10.98907 15.64638

S 10.79085 12.79744 15.20650

S 11.41039 17.35160 14.21710

S 18.58256 10.73730 17.88291

S 16.03231 13.60753 20.62778

S 18.99890 12.63764 13.59297

S 13.94904 13.76453 11.88025

S 18.29924 14.79729 10.39854

S 20.23474 17.63915 13.61968

C 17.06024 22.08783 14.93553

H 17.65601 21.58408 14.14387

H 16.02837 22.23663 14.54400

C 17.67968 23.44360 15.32388

H 17.08342 23.89268 16.15281

H 17.57219 24.12025 14.43987

C 19.13976 23.37720 15.73112

C 20.14763 23.16748 14.76035

H 19.86877 23.06864 13.69125

C 21.50055 23.07955 15.13656

H 22.27323 22.90898 14.36116

C 21.87087 23.21914 16.48960

H 22.93709 23.15811 16.78379

C 20.87800 23.44049 17.46381

H 21.15289 23.56103 18.53050

C 19.52252 23.51078 17.08467

H 18.74357 23.66982 17.85754

C 21.68673 19.79646 18.49764

H 21.48540 20.89174 18.48355

H 21.01551 19.32369 19.24775

C 23.15782 19.50739 18.83827

H 23.35029 18.41371 18.71917

H 23.81876 20.03719 18.11246

C 23.46337 19.95145 20.25693

C 23.97813 21.24032 20.52747

H 24.20964 21.92186 19.68332

C 24.20471 21.66578 21.85106

H 24.62104 22.67447 22.04170

C 23.91055 20.80994 22.93054

H 24.08335 21.14660 23.97031

C 23.39468 19.52389 22.67549

H 23.16168 18.83542 23.51126

C 23.17858 19.10026 21.35106

H 22.78189 18.08242 21.16270

C 20.43574 14.78241 19.67577

H 19.61317 15.49412 19.90925

H 20.15458 13.77783 20.07309

C 21.77540 15.25432 20.26584

H 22.58993 14.57977 19.91002

H 21.99024 16.26516 19.83580

C 21.77588 15.30178 21.77987

C 22.62066 14.44570 22.52394

H 23.29091 13.74681 21.98249

C 22.60632 14.45817 23.93226

H 23.26340 13.76978 24.49892

C 21.74834 15.33689 24.62132

H 21.73289 15.35007 25.72836

C 20.90585 16.20083 23.89194

H 20.22266 16.89083 24.42495

C 20.91752 16.18377 22.48333

H 20.24001 16.85873 21.91792

C 11.73860 21.03292 13.38080

H 11.81690 21.48949 12.36737

H 11.53587 19.94531 13.26626

C 10.61840 21.67582 14.21786

H 10.80690 22.76855 14.34192

H 10.63806 21.21390 15.23587

C 9.27751 21.43424 13.54877

C 8.67055 22.42249 12.73998

H 9.15403 23.41625 12.64032

C 7.45657 22.16577 12.07376

H 6.98842 22.95527 11.45522

C 6.83154 20.91159 12.20472

H 5.87223 20.71261 11.68902

C 7.42636 19.91956 13.01107

H 6.93295 18.93592 13.13370

C 8.63796 20.17682 13.68002

H 9.10070 19.39732 14.32274

C 14.70643 17.63435 10.28980

H 15.10245 16.62756 10.01388

H 13.76510 17.47282 10.85459

C 14.47410 18.48410 9.02347

H 15.45269 18.67642 8.52347

H 13.87179 17.85882 8.32010

C 13.74093 19.79483 9.25077

C 14.44187 21.01386 9.41038

H 15.54962 21.01388 9.36067

C 13.74712 22.22151 9.62217

H 14.31208 23.16637 9.74448

C 12.33961 22.23322 9.67203

H 11.79101 23.18299 9.82907

C 11.63036 21.02596 9.51312

H 10.52333 21.02426 9.55427

C 12.32699 19.82104 9.30086

H 11.75771 18.88099 9.15954

C 13.98882 20.67293 19.25449

H 14.21818 20.33578 20.29283

H 14.94720 20.80730 18.70397

C 13.16397 21.97506 19.24212

H 12.81897 22.14129 18.19187

H 12.24563 21.83196 19.85815

C 13.93015 23.19495 19.71756

C 13.90974 23.59774 21.07327

H 13.33379 22.99682 21.80655

C 14.58891 24.75719 21.49487

H 14.55309 25.05943 22.55913

C 15.29794 25.53958 20.56251

H 15.81084 26.46523 20.88792

C 15.34600 25.13757 19.21240

H 15.90043 25.74585 18.47102

C 14.67480 23.97204 18.79743

H 14.70912 23.65664 17.73440

C 18.15368 20.02471 20.08058

H 19.04161 20.25884 19.44958

H 17.26584 20.41954 19.54051

C 18.30219 20.64736 21.48242

H 17.30583 20.67035 21.98412

H 18.95822 19.99434 22.10495

C 18.90887 22.03741 21.40734

C 20.26141 22.24125 21.76827

H 20.86273 21.38660 22.13980

C 20.85576 23.51369 21.65824

H 21.91505 23.64804 21.95133

C 20.10554 24.60450 21.17938

H 20.57017 25.60602 21.08839

C 18.75829 24.41235 20.81409

H 18.15554 25.26092 20.43838

C 18.16314 23.14168 20.92875

H 17.10056 23.01225 20.63808

C 14.14727 15.96886 22.92935

H 14.69547 15.13148 22.44294

H 14.84491 16.48520 23.62815

C 12.92517 15.41473 23.68638

H 12.44458 16.22777 24.28107

H 12.17214 15.05631 22.94501

C 13.37065 14.26326 24.57227

C 13.16641 12.92365 24.16746

H 12.58488 12.71834 23.24764

C 13.69754 11.85016 24.90897

H 13.53771 10.81066 24.55987

C 14.43945 12.10144 26.07898

H 14.86946 11.26171 26.65842

C 14.62774 13.43012 26.51031

H 15.20324 13.63751 27.43400

C 14.09811 14.49917 25.76302

H 14.25851 15.54160 26.10679

C 12.44349 12.63141 18.90831

H 11.95082 11.91854 18.20561

H 13.53810 12.60323 18.70430

C 12.13240 12.27433 20.37101

H 12.73978 12.95318 21.01922

H 11.05853 12.49178 20.58257

C 12.43135 10.82177 20.70021

C 11.38198 9.91050 20.96570

H 10.33380 10.27318 20.95098

C 11.64720 8.55525 21.24723

H 10.80818 7.86144 21.44675

C 12.97250 8.08149 21.26091

H 13.18167 7.01655 21.47848

C 14.03019 8.97804 21.00414

H 15.07925 8.62015 21.01430

C 13.76326 10.33442 20.73132

H 14.60678 11.03152 20.54192

C 14.96201 9.82890 17.07469

H 14.38339 10.31844 17.88813

H 16.00326 9.66749 17.43845

C 14.32577 8.48362 16.67332

H 14.90680 8.03966 15.83040

H 14.43788 7.79150 17.54471

C 12.86078 8.57001 16.29042

C 11.87194 8.77787 17.28099

H 12.17014 8.85991 18.34558

C 10.51424 8.88161 16.92869

H 9.75733 9.05291 17.71869

C 10.11968 8.75704 15.58147

H 9.04846 8.82063 15.30859

C 11.09399 8.54009 14.58792

H 10.79883 8.43058 13.52589

C 12.45530 8.45844 14.94170

H 13.22007 8.30943 14.15303

C 10.31230 12.18295 13.53008

H 10.47247 11.08090 13.54315

H 11.00304 12.62696 12.78021

C 8.85387 12.52296 13.18323

H 8.70785 13.62602 13.27530

H 8.17099 12.03967 13.92087

C 8.54458 12.05846 11.77302

C 7.98349 10.78524 11.52449

H 7.70433 10.13805 12.38100

C 7.77217 10.33392 10.20686

H 7.32359 9.33715 10.03084

C 8.12564 11.14772 9.11288

H 7.96253 10.79029 8.07741

C 8.68384 12.41986 9.34753

H 8.96714 13.07500 8.50114

C 8.88809 12.86902 10.66504

H 9.32230 13.87421 10.83765

C 11.54398 17.18112 12.38674

H 12.38081 16.48372 12.16469

H 11.81191 18.18692 11.98297

C 10.22419 16.67631 11.78125

H 9.38667 17.32525 12.12864

H 10.03014 15.65775 12.20220

C 10.24513 16.63848 10.26562

C 9.38088 17.47020 9.51607

H 8.68294 18.14535 10.05311

C 9.40644 17.46140 8.10778

H 8.72692 18.12705 7.54119

C 10.29853 16.61415 7.42294

H 10.32274 16.60631 6.31620

C 11.16547 15.77924 8.15731

H 11.87166 15.10970 7.62846

C 11.14062 15.79003 9.56587

H 11.83291 15.13288 10.13496

C 20.25628 10.93871 18.63729

H 20.19482 10.48613 19.65370

H 20.46087 12.02683 18.74102

C 21.35870 10.28825 17.78334

H 21.15976 9.19683 17.66719

H 21.32981 10.74879 16.76524

C 22.71300 10.52339 18.42587

C 23.32594 9.54036 19.23476

H 22.83396 8.55369 19.35678

C 24.55033 9.79620 19.88313

H 25.02436 9.00864 20.50150

C 25.17639 11.04894 19.73820

H 26.13650 11.25452 20.25083

C 24.57363 12.03852 18.93483

H 25.06285 13.02508 18.81163

C 23.35689 11.77610 18.27693

H 22.88912 12.55139 17.63501

C 17.27992 14.35727 21.77209

H 16.90593 15.38498 21.99753

H 18.24312 14.47022 21.23410

C 17.45033 13.53948 23.06764

H 16.45154 13.36033 23.53109

H 18.03209 14.17502 23.77957

C 18.18163 12.22361 22.87709

C 17.48234 11.00429 22.72022

H 16.37442 11.00504 22.76135

C 18.18171 9.79796 22.51978

H 17.61986 8.85179 22.39611

C 19.58956 9.78916 22.48018

H 20.13980 8.84035 22.32805

C 20.29706 10.99757 22.63837

H 21.40456 11.00369 22.60597

C 19.59551 12.20124 22.83831

H 20.15944 13.14577 22.97271

C 18.02960 11.30325 12.76239

H 17.79209 11.66354 11.73394

H 17.07295 11.14124 13.30930

C 18.87738 10.01716 12.73414

H 19.24864 9.83237 13.77133

H 19.77895 10.18772 12.10144

C 18.11811 8.80001 12.24741

C 18.11955 8.42567 10.88357

H 18.67519 9.04647 10.15198

C 17.44014 7.27260 10.44658

H 17.46056 6.99035 9.37525

C 16.75180 6.46696 11.37444

H 16.24234 5.54304 11.03889

C 16.71973 6.84110 12.73301

H 16.17007 6.21739 13.46604

C 17.39309 7.99942 13.16255

H 17.37223 8.28878 14.23310

C 13.86482 11.91904 11.94281

H 12.98841 11.67891 12.58893

H 14.76410 11.52182 12.46231

C 13.69200 11.29742 10.54159

H 14.67946 11.27797 10.02143

H 13.02197 11.94945 9.93347

C 13.08960 9.90414 10.61637

C 11.73706 9.69612 10.25607

H 11.13149 10.54800 9.88539

C 11.14394 8.42317 10.36547

H 10.08340 8.28851 10.07404

C 11.89745 7.33303 10.84161

H 11.43549 6.33035 10.93327

C 13.24572 7.52715 11.20265

H 13.84954 6.67775 11.57592

C 13.83837 8.79940 11.08941

H 14.90076 8.93135 11.37920

C 17.84759 16.03383 9.10000

H 17.30088 16.86974 9.59098

H 17.14743 15.51869 8.40285

C 19.06425 16.59259 8.33831

H 19.54176 15.78304 7.73612

H 19.82231 16.94943 9.07567

C 18.60744 17.74322 7.45793

C 18.79407 19.08179 7.87403

H 19.35306 19.28700 8.80835

C 18.26754 20.15376 7.12837

H 18.42295 21.19227 7.48078

C 17.54591 19.90256 5.94564

H 17.12532 20.74057 5.35718

C 17.36624 18.57451 5.51071

H 16.80344 18.36802 4.58009

C 17.89268 17.50564 6.25989

H 17.74270 16.46310 5.91129

C 19.61939 19.31107 13.13158

H 20.13929 20.02614 13.81340

H 18.52790 19.36547 13.34942

C 19.91330 19.63518 11.65740

H 19.28537 18.95011 11.03716

H 20.97924 19.39868 11.42896

C 19.62634 21.08554 11.31574

C 20.68340 21.98967 11.05513

H 21.72838 21.61776 11.07106

C 20.42723 23.34664 10.77497

H 21.26849 24.03677 10.56694

C 19.10294 23.82558 10.75843

H 18.89881 24.89268 10.54643

C 18.03962 22.93702 11.01848

H 16.99393 23.30453 11.01490

C 18.29729 21.57874 11.28874

H 17.45093 20.88642 11.48199

**$[Au_{25}(PET)_{18}(O_2)_3]^-$ cluster:**

Au 16.03014 18.75615 15.58336

Au 19.04435 19.88525 16.60384

Au 20.85762 16.83549 17.23533

Au 18.30587 14.56014 17.03359

Au 14.54747 17.51485 17.90286

Au 13.17330 20.09952 16.22693

Au 14.67291 19.71564 12.91242

Au 16.22656 16.76724 13.27913

Au 17.63329 17.35290 17.87008

Au 15.85561 17.66367 20.76059

Au 12.83975 15.80827 19.92095

Au 13.45544 14.89602 16.74030

Au 15.95672 13.15084 16.43910

Au 12.86199 12.03988 15.42323

Au 11.10191 15.08613 14.78320

Au 13.71757 17.31454 14.94603

Au 17.44667 14.34369 14.05994

Au 18.79106 11.78917 15.78609

Au 17.31058 12.20710 19.12366

Au 15.79915 15.14022 18.71907

Au 14.37894 14.49830 14.10412

Au 16.13318 14.26483 11.22649

Au 19.16270 16.13940 12.06858

Au 18.55747 16.92899 15.22944

Au 16.00255 15.93896 15.98854

S 16.92055 20.87138 16.36118

S 21.26004 19.12377 16.82466

S 20.61733 14.56131 17.82579

S 13.35552 21.22120 14.16900

S 15.97140 18.37322 11.45515

S 13.02472 19.32501 18.45247

S 18.07425 18.15057 20.12581

S 13.70651 17.20054 21.61957

S 11.77284 14.34144 18.42336

S 14.97542 11.05137 15.72383

S 10.64458 12.81104 15.19136

S 11.41560 17.34392 14.17709

S 18.58204 10.67797 17.85411

S 16.04046 13.57812 20.57718

S 19.09557 12.61425 13.59964

S 13.89744 13.81728 11.81334

S 18.27848 14.75501 10.37056

S 20.24819 17.57126 13.59915

O 15.37963 9.16727 14.00541

O 15.66651 9.72300 12.88510

O 10.04440 18.21165 16.84279

O 10.98274 17.41224 17.16783

O 22.00007 13.61563 15.20557

O 21.06389 14.36198 14.78314

C 17.07709 22.02271 14.92437

H 17.68050 21.53312 14.12966

H 16.04203 22.16104 14.53370

C 17.67884 23.38486 15.32383

H 17.07201 23.82963 16.14821

H 17.56757 24.05822 14.43804

C 19.13824 23.33425 15.73369

C 20.14605 23.12275 14.76295

H 19.86598 23.01882 13.69530

C 21.49975 23.04452 15.13620

H 22.27106 22.86674 14.36112

C 21.87175 23.20072 16.48712

H 22.93884 23.15068 16.78004

C 20.87983 23.42787 17.46103

H 21.15534 23.56517 18.52595

C 19.52282 23.48307 17.08518

H 18.74702 23.64617 17.86032

C 21.72036 19.76579 18.49754

H 21.55822 20.86791 18.46758

H 21.02824 19.33063 19.25196

C 23.17857 19.43353 18.85748

H 23.33417 18.33130 18.76549

H 23.86167 19.92213 18.12343

C 23.49247 19.89964 20.26752

C 24.03715 21.18149 20.51017

H 24.28426 21.83860 19.65199

C 24.27617 21.62987 21.82362

H 24.71780 22.63192 21.99192

C 23.96092 20.80577 22.92164

H 24.14566 21.16076 23.95349

C 23.41155 19.52810 22.69533

H 23.15793 18.86498 23.54590

C 23.18491 19.08092 21.38012

H 22.76399 18.06880 21.21698

C 20.44988 14.75103 19.65092

H 19.61052 15.45163 19.86251

H 20.17975 13.74781 20.06005

C 21.76692 15.26234 20.26411

H 22.61028 14.62307 19.91037

H 21.94958 16.28571 19.84892

C 21.75659 15.29356 21.78013

C 22.59946 14.43101 22.51891

H 23.26763 13.73495 21.97189

C 22.59789 14.44561 23.92734

H 23.26464 13.76061 24.48618

C 21.74801 15.32659 24.62348

H 21.74363 15.33941 25.73076

C 20.89927 16.18904 23.89939

H 20.22550 16.88287 24.43888

C 20.90129 16.17294 22.49046

H 20.22585 16.85339 21.92989

C 11.69399 20.99965 13.39521

H 11.75753 21.47230 12.38825

H 11.51531 19.90981 13.26464

C 10.56399 21.61005 14.24293

H 10.74215 22.70199 14.38871

H 10.57939 21.12790 15.25026

C 9.22963 21.36939 13.56174

C 8.67605 22.32020 12.67423

H 9.20003 23.28448 12.51655

C 7.47311 22.05821 11.99091

H 7.05062 22.81925 11.30541

C 6.80596 20.83291 12.18245

H 5.86074 20.62377 11.64522

C 7.34689 19.87817 13.06787

H 6.82478 18.91634 13.23556

C 8.54643 20.14523 13.75454

H 8.96822 19.39412 14.45536

C 14.72755 17.61483 10.31005

H 15.12901 16.60264 10.06243

H 13.77792 17.46125 10.86378

C 14.50722 18.43719 9.02412

H 15.49104 18.63832 8.53700

H 13.92224 17.78894 8.32596

C 13.75888 19.74015 9.23507

C 14.45238 20.96151 9.40329

H 15.55968 20.96376 9.35081

C 13.75260 22.16413 9.62332

H 14.31330 23.11159 9.74863

C 12.34506 22.16618 9.67739

H 11.79252 23.11111 9.84761

C 11.64198 20.95660 9.50643

H 10.53447 20.94545 9.54620

C 12.34474 19.75686 9.28477

H 11.77908 18.81560 9.13632

C 14.02308 20.66567 19.24635

H 14.28402 20.31551 20.27323

H 14.96592 20.81601 18.67282

C 13.18269 21.95791 19.28213

H 12.78995 22.13359 18.25041

H 12.29597 21.79639 19.93932

C 13.95398 23.18129 19.73600

C 13.92835 23.60950 21.08337

H 13.34435 23.02839 21.82528

C 14.61055 24.77229 21.48845

H 14.56772 25.09740 22.54594

C 15.33256 25.53034 20.54689

H 15.85395 26.45580 20.85913

C 15.38528 25.10418 19.20421

H 15.95002 25.69658 18.45791

C 14.70554 23.93880 18.80509

H 14.73705 23.61192 17.74544

C 18.17700 19.99150 20.06315

H 19.04977 20.21987 19.40814

H 17.27773 20.40078 19.55211

C 18.37120 20.59695 21.46692

H 17.39374 20.59119 22.00694

H 19.06418 19.94477 22.04884

C 18.95285 21.99799 21.40099

C 20.30921 22.21734 21.73635

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Au 15.91244 17.68559 20.7804**8**

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Au 13.45313 14.95172 16.77100

Au 15.94053 13.18951 16.47788

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C 18.31273 21.42900 11.16875

H 17.47600 20.72204 11.34702

O 16.35645 22.20128 19.21558

O 16.78990 22.80619 18.17650

O 15.39328 9.18677 14.00712

O 15.73286 9.76651 12.91563

O 9.98608 18.20954 16.79035

O 11.00238 17.57540 17.21112

O 22.01159 13.59404 15.21714

O 21.01200 14.24215 14.78249

**$[Au_{25}(PET)_{18}(O_2)]^-$ cluster using vdw-DF2 functional**

Au 15.54188 18.90001 15.59014

Au 12.55064 19.78081 17.10935

Au 11.76473 16.70148 19.15091

Au 14.11785 14.38176 17.71113

Au 14.90713 16.69198 13.37662

Au 16.44488 19.87292 12.55371

Au 18.30990 20.79570 15.75627

Au 17.72647 17.87928 17.52419

Au 13.08598 16.73175 15.98516

Au 11.80585 15.85490 12.68717

Au 14.83302 14.14114 11.23348

Au 17.27207 14.61523 13.82787

Au 16.45289 13.18149 16.53351

Au 19.43437 12.23285 14.91693

Au 20.18178 15.27667 12.84503

Au 17.83060 17.67158 14.36301

Au 17.05203 15.35280 18.73080

Au 15.60375 12.22461 19.55660

Au 13.66702 11.30482 16.34915

Au 14.22119 14.19126 14.56582

Au 18.90694 15.34715 16.05008

Au 20.08899 16.20505 19.39822

Au 17.02643 17.90836 20.85120

Au 14.69988 17.41582 18.27314

Au 15.98762 16.02835 16.05092

S 13.77235 20.64880 15.19187

S 11.24328 19.07155 19.01919

S 12.09335 14.30050 19.20831

S 17.64838 21.70560 13.60176

S 19.02705 20.00026 17.94441

S 15.08478 18.21551 11.40500

S 10.87122 16.61866 14.77952

S 12.60651 14.89972 10.59953

S 17.04969 13.27759 11.67811

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S 20.75608 12.92396 13.00754

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S 14.81310 18.78949 20.39922

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## References


1. Gong, J.; Mullins, C. B. Surface Science Investigations of Oxidative Chemistry on Gold. *Acc. Chem. Res.* **2009**, *42*, 1063-1073.
2. Kim, J.; Samano, E.; Koel, B. E. Oxygen Adsorption and Oxidation Reactions on Au(2 1 1) Surfaces: Exposures Using $O_2$ at High Pressures and Ozone ($O_3$) in UHV. *Surf. Sci.* **2006**, *600*, 4622-4632.
3. Xu, Y.; Mavrikakis, M. Adsorption and Dissociation of $O_2$ on Gold Surfaces: Effect of Steps and Strain. *J. Phys. Chem. B* **2003**, *107*, 9298-9307.
4. Okamoto, Y. Density-functional Calculations of Atomic and Molecular Adsorptions on 55-atom Metal Clusters: Comparison with (1 1 1) Surfaces. *Chem. Phys. Lett.* **2005**, *405*, 79-83.
5. Roldan, A.; Ricart, J. M.; Illas, F.; Pacchioni, G. $O_2$ Adsorption and Dissociation on Neutral, Positively and Negatively Charged $Au_n$ (n = 5-79) clusters. *Phys. Chem. Chem. Phys.* **2010**, *12*, 10723-10729.