Supporting Information

for the manuscript

Oxygen Activation on Nanometer-size Gold Nanoparticles

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Table 1

Atomic Cartesian coordinates of Au₁₀. All values are in Å.

Au	-0.820506000	0.081070000	-0.347835000
Au	0.955002000	0.041423000	1.878159000
Au	-2.933426000	-1.863328000	-0.260597000
Au	-2.759032000	-0.127879000	-2.423731000
Au	-1.140274000	-1.782614000	1.813858000
Au	-0.529884000	1.870650000	-2.443484000
Au	1.220975000	1.952107000	-0.416200000
Au	-2.481372000	1.600087000	-4.451013000
Au	-3.185607000	-3.624600000	1.837494000
Au	2.926753000	1.853084000	1.816565000

Table 2

Atomic Cartesian coordinates of Au₁₈. All values are in Å.

Au	-0.230232000	-2.333057000	-2.073447000
Au	1.332260000	-4.335886000	-3.589809000
Au	1.250497000	0.089187000	-1.352030000
Au	-0.726169000	-0.693579000	0.306406000
Au	2.217635000	-1.747225000	-3.473947000
Au	-1.930057000	-3.389714000	-0.002940000
Au	-0.861646000	-5.203772000	-1.755251000
Au	3.382357000	0.743578000	-3.073545000
Au	-2.723071000	-1.675696000	2.034156000
Au	3.983800000	-1.024426000	-1.017321000
Au	3.153059000	-3.864650000	-1.552853000
Au	1.758183000	-6.428241000	-1.637358000
Au	0.631411000	-4.863720000	0.555097000
Au	-0.162407000	-2.668897000	2.452010000
Au	2.014412000	-1.417106000	1.044346000
Au	2.265890000	-3.927236000	2.589058000
Au	3.411776000	-5.753142000	0.661540000
Au	4.458730000	-3.057242000	0.755425000

Table 3

Atomic Cartesian coordinates of Au₂₀. All values are in Å.

Au	0.069400000	-2.481367000	-1.786653000
Au	1.250141000	-4.289737000	-3.735791000
Au	1.243732000	0.145302000	-1.360656000
Au	-0.759171000	-0.649178000	0.314437000
Au	2.308957000	-1.784070000	-3.506561000
Au	-1.950494000	-3.472923000	0.058300000
Au	-1.006448000	-5.183745000	-1.847309000
Au	3.367177000	0.765741000	-3.069775000
Au	-2.728494000	-1.649230000	2.028077000
Au	0.145305000	-6.857786000	-3.767816000
Au	4.056128000	-1.069636000	-1.077572000
Au	3.022321000	-3.757227000	-1.491553000
Au	1.804048000	-6.398129000	-1.566511000
Au	0.651730000	-4.697116000	0.493082000
Au	-0.203652000	-2.758303000	2.485616000
Au	1.904203000	-1.731124000	0.762967000
Au	2.291967000	-3.835162000	2.734530000
Au	3.355778000	-5.764191000	0.587604000
Au	4.549107000	-2.940729000	0.847304000
Au	4.863568000	-4.928421000	2.787971000

Table 4

Atomic Cartesian coordinates of Au₂₄. All values are in Å.

Au	-0.679013000	-1.692847000	-2.745194000
Au	4.217370000	-2.577994000	-3.095587000
Au	-0.560198000	-2.141603000	0.094594000
Au	1.706608000	-1.914488000	-4.340450000
Au	4.336184000	-3.026748000	-0.255799000
Au	1.950564000	-2.805108000	1.339457000
Au	3.100118000	-5.352776000	0.815833000
Au	3.556230000	-5.153487000	-2.013760000
Au	2.867355000	-4.482024000	-4.719391000
Au	0.197451000	-4.261828000	-3.682611000
Au	-1.782369000	-4.057773000	-1.615972000
Au	0.360627000	-4.857886000	0.118638000
Au	1.728335000	-6.778311000	-3.655813000
Au	-0.666538000	-6.560180000	-2.054398000
Au	1.850403000	-7.228064000	-0.802993000
Au	3.459721000	-0.457768000	0.681619000
Au	0.789817000	-0.237571000	1.718397000
Au	0.100940000	0.433891000	-0.987233000
Au	0.557054000	0.633180000	-3.816826000
Au	3.296546000	0.138291000	-3.119633000
Au	5.439540000	-0.661822000	-1.385022000
Au	4.323710000	1.840585000	-0.946595000
Au	1.806769000	2.508469000	-2.198000000
Au	1.928838000	2.058716000	0.654820000

Table 5

Atomic Cartesian coordinates of Au₃₈. All values are in Å.

Au	-2.085679000	-0.128596000	4.332174000
Au	2.153613000	0.004986000	4.353247000
Au	4.126756000	-0.018529000	2.120718000
Au	2.017975000	-0.024640000	0.044200000
Au	0.041907000	-0.093570000	2.175814000
Au	0.077511000	1.932780000	4.153389000
Au	2.309573000	2.192572000	2.320426000
Au	-4.052521000	-0.011064000	2.055365000
Au	-2.018532000	0.029004000	-0.061104000
Au	-0.046425000	0.095929000	-2.130394000
Au	-0.030561000	1.971050000	-0.095943000
Au	-2.246087000	2.177789000	2.319133000
Au	0.034772000	-1.965251000	0.146122000
Au	-2.254423000	-2.245449000	2.354055000
Au	2.244212000	-2.218003000	2.394047000
Au	-0.046057000	-2.101900000	4.308800000
Au	-2.372400000	-2.232418000	-2.377348000
Au	-4.063297000	-1.938983000	-0.075394000
Au	-4.092788000	1.997840000	-0.049104000
Au	-2.305054000	2.232508000	-2.385058000
Au	-2.129771000	0.002728000	-4.251752000
Au	-4.282809000	0.032088000	-2.181545000
Au	4.217879000	-0.016714000	-2.111633000
Au	2.033748000	0.074172000	-4.184169000
Au	4.099744000	-2.010359000	0.012813000
Au	2.309839000	-2.190531000	-2.310560000
Au	-0.086981000	-1.969400000	-4.138244000
Au	0.055281000	2.105741000	-4.246413000
Au	2.328080000	2.304839000	-2.394960000
Au	4.043515000	1.944458000	-0.018333000

Au	-2.046225000	4.024615000	-0.075731000
Au	-0.009167000	3.955198000	2.010272000
Au	1.980540000	3.991616000	-0.090894000
Au	-0.022725000	4.131551000	-2.191225000
Au	0.021293000	-4.108713000	2.177990000
Au	2.062876000	-4.031449000	0.069232000
Au	0.026503000	-3.931689000	-2.000205000
Au	-1.994111000	-3.964205000	0.022208000

Table 6

Atomic Cartesian coordinates of Au₄₂. All values are in Å.

Au	2.148106000	-4.143112000	0.000000000
Au	0.001370000	-6.111133000	0.000000000
Au	-2.148061000	-4.146183000	0.000000000
Au	-4.143121000	-2.147978000	0.000000000
Au	-2.056154000	0.001221000	0.000000000
Au	-0.001652000	-2.055958000	0.000000000
Au	-0.000812000	-4.121115000	-2.072935000
Au	-2.278429000	-2.278413000	-2.247521000
Au	4.146116000	-2.147958000	0.000000000
Au	2.055731000	-0.001558000	0.000000000
Au	0.001080000	2.055678000	0.000000000
Au	-0.000164000	-0.000124000	-2.004257000
Au	2.278404000	-2.278416000	-2.247501000
Au	-0.000164000	-0.000124000	2.004257000
Au	2.278404000	-2.278416000	2.247501000
Au	-2.278429000	-2.278413000	2.247521000
Au	-0.000812000	-4.121115000	2.072935000
Au	2.278445000	2.278369000	2.247529000
Au	4.121184000	-0.000862000	2.072900000
Au	4.121184000	-0.000862000	-2.072900000
Au	2.278445000	2.278369000	-2.247529000
Au	6.111297000	0.001417000	0.000000000
Au	2.148075000	4.146047000	0.000000000
Au	4.143167000	2.148018000	0.000000000
Au	-6.110877000	-0.000948000	0.000000000
Au	-4.146114000	2.148286000	0.000000000
Au	-2.147843000	4.143104000	0.000000000
Au	-0.001042000	6.111369000	0.000000000
Au	-4.121167000	0.000932000	2.072994000
Au	-2.278354000	2.278475000	2.247544000

Au	0.000914000	4.121110000	2.072911000
Au	0.000914000	4.121110000	-2.072911000
Au	-2.278354000	2.278475000	-2.247544000
Au	-4.121167000	0.000932000	-2.072994000
Au	2.092573000	-0.000548000	-4.060197000
Au	-0.000523000	-2.092660000	-4.060166000
Au	-2.092620000	0.000519000	-4.060207000
Au	0.000509000	2.092579000	-4.060185000
Au	-0.000523000	-2.092660000	4.060166000
Au	-2.092620000	0.000519000	4.060207000
Au	0.000509000	2.092579000	4.060185000
Au	2.092573000	-0.000548000	4.060197000