Dissociative Chemisorption of O_2 on Ag_n and $Ag_{n-1}Ir$ (n=3-26) Clusters: A First-principle Study

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Supporting Information

TableS1. The average Ag-Ag CN and average Ag-Ag bond length for Ag_n clusters.

TableS2. The average Ag-Ag CN and average Ag-Ag bond length for $Ag_{n-1}Ir$ clusters.

TableS3. The average Ag-Ir CN and average Ag-Ir bond length for $Ag_{n-1}Ir$ clusters.

TableS4. The E_b values for Ag_n and $Ag_{n-1}Ir$ clusters.

TableS5. The Δ_2E and E^{mon}, E^{dim}, values for Ag_n and $Ag_{n-1}Ir$ clusters.

TableS6. The $E_{HOMO-LOMO}$ values for Ag_n and $Ag_{n-1}Ir$ clusters.

TableS7 The O_2 adsorption energy, the Bader charge of O_2 (Q_{O2}), Ag (Q_{Ag}), the bond length of O-O bond for O_2 adsorption on Ag_n.

TableS8 The O_2 adsorption energy, the Bader charge of O_2 (Q_{O2}), Ag (Q_{Ag}), Ir (Q_{Ir}), the bond length of O-O bond for O_2 adsorption on $Ag_{n-1}Ir$

TableS9. The O_2 dissociation barriers and the O-O distance (b) of the transition states of O_2 adsorption on Ag_n and $Ag_{n-1}Ir$ (n = 3–26) clusters.

TableS10. K and k (s^{-1}) are the equilibrium constant and O_2 direct dissociation rate constant, respectively. θ_{O2} and θ* are the coverages of O_2 and free sites of the clusters. r (molecules·s^{-1} ·site^{-1}) for O_2 direct dissociation process at T=600 K and P_{O2} =3×10^{-5}Pa.

TableS11. K and k (s^{-1}) are the equilibrium constant and O_2 direct dissociation rate constant, respectively. θ_{O2} and θ* are the coverages of O_2 and free sites of the clusters. r (molecules·s^{-1} ·site^{-1}) stand for the reaction rate for O_2 direct dissociation process at T=600 K and P_{O2} =3×10^{-4}Pa.

TableS12. The bond length, coordination numbers (CN), E^{mon}, E^{dim}, O_2 adsorption energy (E_{ads}) of Ag_{10}, Ag_8Ir for PBE and TPSS functional.

Fig. S1 : Total densities of states of two typical clusters : Ag_6 and Ag_5Ir clusters.

TableS1. The average Ag-Ag CN and average Ag-Ag bond length for Ag_n clusters.

Ag_n	2S+1	CN(Ag-Ag)	R(Ag-Ag)/Å	Ag_n	2S+1	CN(Ag-Ag)	R(Ag-Ag)/Å
Ag_3	2	2.00	2.79	Ag_{15}	2	5.73	2.85
Ag_4	1	2.50	2.73	Ag_{16}	1	6.00	2.87
Ag_5	2	2.80	2.74	Ag_{17}	2	5.29	2.82
Ag_6	1	3.00	2.74	Ag_{18}	1	6.33	2.86
Ag_7	2	4.57	2.82	Ag_{19}	2	6.32	2.87
Ag_8	1	4.50	2.81	Ag_{20}	1	6.30	2.86
Ag_9	2	4.67	2.82	Ag_{21}	2	6.38	2.87
Ag_{10}	1	4.80	2.83	Ag_{22}	1	7.09	2.91
Ag_{11}	2	5.45	2.85	Ag_{23}	2	7.13	2.91
Ag_{12}	1	5.67	2.85	Ag_{24}	1	6.75	2.88
Ag_{13}	2	5.85	2.86	Ag_{25}	2	7.28	2.88
Ag_{14}	1	6.00	2.87	Ag_{26}	1	6.77	2.88

TableS2. The average Ag-Ag CN and average Ag-Ag bond length for $Ag_{n-1}Ir$ clusters.

$Ag_{n-1}Ir$	2S+1	CN(Ag-Ag)	R(Ag-Ag)/Å	$Ag_{n-1}Ir$	2S+1	CN(Ag-Ag)	R(Ag-Ag)/Å
Ag_2Ir	2	1.00	2.98	$Ag_{14}Ir$	2	5.14	2.89
Ag_3Ir	3	0.67	2.71	$Ag_{15}Ir$	1	5.3	2.90
Ag_4Ir	2	1.50	2.79	$Ag_{16}Ir$	2	5.63	2.90
Ag_5Ir	1	2.00	2.84	$Ag_{17}Ir$	1	5.76	2.90
Ag_6Ir	2	2.00	2.74	$Ag_{18}Ir$	2	6.00	2.91
Ag_7Ir	1	2.57	2.81	$Ag_{19}Ir$	1	6.00	2.91
Ag_8Ir	2	3.75	2.92	$Ag_{20}Ir$	2	6.40	2.92
Ag_9Ir	3	3.78	2.99	$Ag_{21}Ir$	1	6.48	2.92
$Ag_{10}Ir$	2	4.20	2.94	$Ag_{22}Ir$	2	6.55	2.91
$Ag_{11}Ir$	1	4.18	2.88	$Ag_{23}Ir$	1	6.61	2.92
$Ag_{12}Ir$	2	4.67	2.89	$Ag_{24}Ir$	2	6.50	2.91

$Ag_{13}Ir$	1	4.92	2.89	$Ag_{25}Ir$	1	6.32	2.89

TableS3. The average Ag-Ir CN and average Ag-Ir bond length for $Ag_{n-1}Ir$ clusters.

$Ag_{n-1}Ir$	CN(Ag-Ir)	R(Ag-Ir)/Å	$Ag_{n-1}Ir$	CN(Ag-Ir)	R(Ag-Ir)/Å
Ag_2Ir	1.00	2.55	$Ag_{14}Ir$	0.79	2.75
Ag_3Ir	1.00	2.62	$Ag_{15}Ir$	0.73	2.76
Ag_4Ir	1.00	2.64	$Ag_{16}Ir$	0.75	2.79
Ag_5Ir	1.00	2.63	$Ag_{17}Ir$	0.71	2.79
Ag_6Ir	1.00	2.69	$Ag_{18}Ir$	0.67	2.78
Ag_7Ir	1.00	2.68	$Ag_{19}Ir$	0.63	2.78
Ag_8Ir	1.00	2.68	$Ag_{20}Ir$	0.6	2.77
Ag_9Ir	1.00	2.65	$Ag_{21}Ir$	0.52	2.79
$Ag_{10}Ir$	1.00	2.70	$Ag_{22}Ir$	0.55	2.78
$Ag_{11}Ir$	0.91	2.72	$Ag_{23}Ir$	0.48	2.79
$Ag_{12}Ir$	0.92	2.75	$Ag_{24}Ir$	0.5	2.78
$Ag_{13}Ir$	0.85	2.75	$Ag_{25}Ir$	0.48	2.79

TableS4. The E_b values for Ag_n and $Ag_{n-1}Ir$ clusters.

Ag_n	E_b(eV)	$Ag_{n-1}Ir$	E_b(eV)	Ag_n	E_b(eV)	$Ag_{n-1}Ir$	E_b(eV)
Ag_3	0.89	Ag_2Ir	1.54	Ag_{15}	1.71	$Ag_{14}Ir$	2.05
Ag_4	1.17	Ag_3Ir	1.62	Ag_{16}	1.74	$Ag_{15}Ir$	2.06
Ag_5	1.27	Ag_4Ir	1.75	Ag_{17}	1.76	$Ag_{16}Ir$	2.06
Ag_6	1.44	Ag_5Ir	1.80	Ag_{18}	1.80	$Ag_{17}Ir$	2.07
Ag_7	1.46	Ag_6Ir	1.95	Ag_{19}	1.81	$Ag_{18}Ir$	2.06
Ag_8	1.56	Ag_7Ir	1.98	Ag_{20}	1.83	$Ag_{19}Ir$	2.07
Ag_9	1.53	Ag_8Ir	2.04	Ag_{21}	1.82	$Ag_{20}Ir$	2.08
Ag_{10}	1.59	Ag_9Ir	2.09	Ag_{22}	1.83	$Ag_{21}Ir$	2.09
Ag_{11}	1.60	$Ag_{10}Ir$	2.06	Ag_{23}	1.83	$Ag_{22}Ir$	2.08
Ag_{12}	1.65	$Ag_{11}Ir$	2.06	Ag_{24}	1.85	$Ag_{23}Ir$	2.08
Ag_{13}	1.66	$Ag_{12}Ir$	2.04	Ag_{25}	1.85	$Ag_{24}Ir$	2.07

Ag_{14}	1.71	$Ag_{13}Ir$	2.05	Ag_{26}	1.87	$Ag_{25}Ir$	2.07

TableS5. The Δ_2E and E^{mon}, E^{dim}, values for Ag_n and $Ag_{n-1}Ir$ clusters.

Ag_n	Δ_2E(eV)	E_{Ag1}^{mon}(eV)	E_{Ag2}^{dim}(eV)	$Ag_{n-1}Ir$	Δ_2E(eV)	E_{Ag1}^{mon}(eV)	E_{Ag2}^{dim}(eV)	E_{Ir}^{mon}(eV)	E_{AgIr}^{dim}(eV)
Ag_3	-1.14	0.86	0.86	Ag_2Ir	0.21	2.09	2.81	2.81	2.09
Ag_4	0.31	2.00	1.06	Ag_3Ir	-0.38	1.88	2.16	3.83	1.91
Ag_5	-0.60	1.69	1.89	Ag_4Ir	0.21	2.25	2.33	4.08	3.30
Ag_6	0.68	2.28	2.17	Ag_5Ir	-0.85	2.04	2.50	4.44	3.34
Ag_7	-0.66	1.60	2.08	Ag_6Ir	0.75	2.89	3.13	5.05	4.55
Ag_8	0.93	2.26	2.05	Ag_7Ir	-0.39	2.14	3.23	5.58	4.40
Ag_9	-0.57	1.32	1.78	Ag_8Ir	-0.07	2.53	2.87	5.86	5.33
Ag_{10}	0.39	2.11	1.63	Ag_9Ir	0.94	2.60	3.33	7.14	5.68
Ag_{11}	-0.43	1.73	2.04	$Ag_{10}Ir$	-0.46	1.66	2.46	6.91	6.02
Ag_{12}	0.32	2.15	2.08	$Ag_{11}Ir$	0.29	2.12	1.98	7.09	6.25
Ag_{13}	-0.52	1.84	2.19	$Ag_{12}Ir$	-0.36	1.83	2.15	6.76	6.14
Ag_{14}	0.65	2.36	2.39	$Ag_{13}Ir$	0.22	2.19	2.21	7.15	6.17
Ag_{15}	-0.46	1.71	2.26	$Ag_{14}Ir$	-0.20	1.97	2.33	6.72	6.33
Ag_{16}	0.10	2.17	2.07	$Ag_{15}Ir$	0.03	2.17	2.33	7.18	6.10
Ag_{17}	-0.31	2.07	2.43	$Ag_{16}Ir$	-0.03	2.14	2.50	7.27	6.54
Ag_1	0.37	2.38	2.65	$Ag_{17}Ir$	0.16	2.17	2.51	7.37	6.66

Ag_{18}									
Ag_{19}	-0.34	2.01	2.59	$Ag_{18}Ir$	-0.23	2.01	2.38	6.89	6.60
Ag_{20}	0.81	2.35	2.56	$Ag_{19}Ir$	0.04	2.24	2.45	7.12	6.35
Ag_{21}	-0.54	1.55	2.10	$Ag_{20}Ir$	-0.13	2.19	2.63	6.96	6.53
Ag_{22}	0.27	2.09	1.83	$Ag_{21}Ir$	0.51	2.32	2.72	7.75	6.50
Ag_{23}	-0.37	1.82	2.11	$Ag_{22}Ir$	-0.31	1.81	2.34	7.45	6.79
Ag_{24}	0.27	2.19	2.21	$Ag_{23}Ir$	0.24	2.13	2.14	7.76	6.80
Ag_{25}	-0.56	1.91	2.30	$Ag_{24}Ir$	-0.23	1.88	2.21	7.47	6.87
Ag_{26}		2.48	2.59	$Ag_{25}Ir$		2.11	2.19	7.74	6.80

TableS6. The $E_{HOMO-LOMO}$ values for Ag_n and $Ag_{n-1}Ir$ clusters.

Ag_n	$E_{HOMO-LOMO}$(eV)	$Ag_{n-1}Ir$	$E_{HOMO-LOMO}$(eV)	Ag_n	$E_{HOMO-LOMO}$(eV)	$Ag_{n-1}Ir$	$E_{HOMO-LOMO}$(eV)
Ag_3	0.31	Ag_2Ir	0.31	Ag_{15}	0.18	$Ag_{14}Ir$	0.20
Ag_4	0.84	Ag_3Ir	0.01	Ag_{16}	0.68	$Ag_{15}Ir$	0.72
Ag_5	0.38	Ag_4Ir	0.22	Ag_{17}	0.16	$Ag_{16}Ir$	0.32

Ag_6	2.21	Ag_5Ir	0.28	Ag_{18}	0.76	$Ag_{17}Ir$	0.64
Ag_7	0.34	Ag_6Ir	0.65	Ag_{19}	0.16	$Ag_{18}Ir$	0.22
Ag_8	2.32	Ag_7Ir	0.75	Ag_{20}	1.15	$Ag_{19}Ir$	0.66
Ag_9	0.27	Ag_8Ir	0.69	Ag_{21}	0.15	$Ag_{20}Ir$	0.22
Ag_{10}	1.11	Ag_9Ir	1.64	Ag_{22}	0.53	$Ag_{21}Ir$	0.66
Ag_{11}	0.21	$Ag_{10}Ir$	0.16	Ag_{23}	0.15	$Ag_{22}Ir$	0.19
Ag_{12}	0.88	$Ag_{11}Ir$	0.85	Ag_{24}	0.75	$Ag_{23}Ir$	0.91
Ag_{13}	0.18	$Ag_{12}Ir$	0.15	Ag_{25}	0.13	$Ag_{24}Ir$	0.17
Ag_{14}	1.11	$Ag_{13}Ir$	0.53	Ag_{26}	0.82	$Ag_{25}Ir$	0.66

TableS7 The O_2 adsorption energy, the Bader charge of O_2 (Q_{O2}), Ag (Q_{Ag}), the bond length of O-O bond for O_2 adsorption on Ag_n.

O_2/Ag_n	E_{ads}(eV)	Q_{O2}(eV)	Q_{Ag}(eV)	R_{O-O}(Å)
O_2/Ag_3	1.18	-0.53	0.53	1.33
O_2/Ag_4	0.43	-0.53	0.53	1.32
O_2/Ag_5	0.98	-0.61	0.61	1.34
O_2/Ag_6	0.17	-0.21	0.21	1.25
O_2/Ag_7	0.78	-0.01	0.01	1.32
O_2/Ag_8	0.19	-0.20	0.20	1.26
O_2/Ag_9	0.90	-0.58	0.58	1.34
O_2/Ag_{10}	0.57	0.01	-0.01	1.31

O_2/Ag_{11}	0.68	-0.37	0.37	1.34
O_2/Ag_{12}	0.45	-0.44	0.44	1.30
O_2/Ag_{13}	0.73	-0.58	0.58	1.33
O_2/Ag_{14}	0.05	0.07	-0.07	1.31
O_2/Ag_{15}	0.62	-0.52	0.52	1.32
O_2/Ag_{16}	0.32	-0.52	0.52	1.32
O_2/Ag_{17}	0.32	-0.06	0.06	1.33
O_2/Ag_{18}	0.18	-0.25	0.25	1.30
O_2/Ag_{19}	0.34	-0.56	0.56	1.33
O_2/Ag_{20}	0.11	-0.16	0.16	1.31
O_2/Ag_{21}	0.62	-0.55	0.55	1.32
O_2/Ag_{22}	0.42	-0.43	0.43	1.32
O_2/Ag_{23}	0.71	-0.28	0.28	1.33
O_2/Ag_{24}	0.31	-0.52	0.52	1.31
O_2/Ag_{25}	0.58	-0.42	0.42	1.35
O_2/Ag_{26}	0.23	-0.48	0.48	1.30

TableS8 The O_2 adsorption energy, the Bader charge of O_2 (Q_{O2}), Ag (Q_{Ag}), Ir (Q_{Ir}), the bond length of O-O bond for O_2 adsorption on $Ag_{n-1}Ir$

$O_2/Ag_{n-1}Ir$	E_{ads}(eV)	Q_{O2}(eV)	Q_{Ag}(eV)	Q_{Ir}(eV)	R_{O-O}(Å)
O_2/Ag_2Ir	2.71	-0.59	0.17	0.42	1.39
O_2/Ag_3Ir	2.37	-0.49	0.19	0.30	1.29
O_2/Ag_4Ir	1.93	-0.60	0.32	0.28	1.37
O_2/Ag_5Ir	2.46	-0.53	0.28	0.25	1.29
O_2/Ag_6Ir	1.49	-0.54	0.33	0.21	1.32
O_2/Ag_7Ir	1.93	-0.65	0.45	0.20	1.36
O_2/Ag_8Ir	1.38	-0.66	0.53	0.13	1.37
O_2/Ag_9Ir	0.41	-0.82	0.66	0.16	1.42
$O_2/Ag_{10}Ir$	1.26	-0.59	0.79	-0.20	1.33
$O_2/Ag_{11}Ir$	0.56	-0.52	0.74	-0.22	1.32

$O_2/Ag_{12}Ir$	1.10	-0.01	0.32	-0.31	1.34
$O_2/Ag_{13}Ir$	0.71	-0.41	0.08	-0.49	1.34
$O_2/Ag_{14}Ir$	0.98	-1.04	1.14	-0.10	1.33
$O_2/Ag_{15}Ir$	0.43	-0.35	0.64	-0.29	1.33
$O_2/Ag_{16}Ir$	0.64	-0.57	0.79	-0.22	1.33
$O_2/Ag_{17}Ir$	0.47	-0.56	0.78	-0.22	1.32
$O_2/Ag_{18}Ir$	0.71	-0.65	0.86	-0.21	1.32
$O_2/Ag_{19}Ir$	0.45	-0.51	0.77	-0.26	1.33
$O_2/Ag_{20}Ir$	0.76	-0.60	0.85	-0.25	1.34
$O_2/Ag_{21}Ir$	0.39	-0.54	0.76	-0.22	1.28
$O_2/Ag_{22}Ir$	0.89	-0.57	0.83	-0.26	1.32
$O_2/Ag_{23}Ir$	0.41	-0.38	0.68	-0.30	1.31
$O_2/Ag_{24}Ir$	0.73	-0.68	0.92	-0.24	1.34
$O_2/Ag_{25}Ir$	0.34	0.04	0.31	-0.35	1.31

TableS9. The O_2 dissociation barriers and the O-O distance (b) of the transition states of O_2 adsorption on Ag_n and $Ag_{n-1}Ir$ (n = 3–26) clusters.

Ag_n	Barrier(eV)	R(O-O) /Å	$Ag_{n-1}Ir$	Barrier(eV)	R(O-O) /Å
Ag_3	2.41	2.39	Ag_2Ir	0.80	1.81
Ag_4	1.96	2.58	Ag_3Ir	0.89	1.88
Ag_5	2.33	2.54	Ag_4Ir	0.56	1.88
Ag_6	2.35	2.31	Ag_5Ir	0.73	1.77
Ag_7	1.94	1.80	Ag_6Ir	0.58	2.03
Ag_8	2.09	2.24	Ag_7Ir	0.77	2.18
Ag_9	1.59	2.04	Ag_8Ir	0.34	1.96
Ag_{10}	1.37	2.02	Ag_9Ir	0.53	1.77
Ag_{11}	2.47	2.21	$Ag_{10}Ir$	2.00	2.49
Ag_{14}	1.42	1.91	$Ag_{13}Ir$	1.47	2.12
Ag_{18}	1.42	1.89	$Ag_{17}Ir$	1.41	1.97
Ag_{19}	1.71	1.97	$Ag_{18}Ir$	2.02	2.02
Ag_{20}	1.54	1.85	$Ag_{19}Ir$	1.59	1.99
Ag_{25}	1.81	1.98	$Ag_{24}Ir$	1.55	1.92
Ag_{26}	1.49	1.96	$Ag_{25}Ir$	1.30	1.96

TableS10. K and k (s^{-1}) are the equilibrium constant and O_2 direct dissociation rate constant, respectively. θ_{O2} and θ^* are the coverages of O_2 and free sites of the clusters. r (molecules·s^{-1} ·$site^{-1}$) for O_2 direct dissociation process at T=600 K and P_{O2} =3×10^{-5}Pa.

Ag_n						
Clusters	K	k	θ_{O_2}	θ_*	$\theta_{O_2} * \theta_*$	r
Ag_3	4.0×10^{-6}	1.5×10^{-7}	1.2×10^{-10}	1	1.2×10^{-10}	1.8×10^{-17}
Ag_4	2.1×10^{-12}	4.4×10^{-4}	6.4×10^{-17}	1	6.4×10^{-17}	2.8×10^{-20}
Ag_5	8.5×10^{-8}	3.4×10^{-7}	2.6×10^{-12}	1	2.6×10^{-12}	8.8×10^{-19}
Ag_6	1.4×10^{-14}	7.0×10^{-7}	4.2×10^{-19}	1	4.2×10^{-19}	2.9×10^{-25}
Ag_7	1.8×10^{-9}	7.6×10^{-4}	5.4×10^{-14}	1	5.4×10^{-14}	4.1×10^{-17}
Ag_8	2.1×10^{-14}	9.9×10^{-5}	6.2×10^{-19}	1	6.2×10^{-19}	6.2×10^{-23}
Ag_9	1.8×10^{-8}	3.4	5.5×10^{-13}	1	5.5×10^{-13}	1.9×10^{-12}
Ag_{10}	3.1×10^{-11}	0.60	9.4×10^{-16}	1	9.4×10^{-16}	5.7×10^{-16}
Ag_{11}	2.6×10^{-10}	3.8×10^{-9}	7.9×10^{-15}	1	7.9×10^{-15}	3.0×10^{-23}
Ag_{14}	1.4×10^{-15}	12	4.2×10^{-20}	1	4.2×10^{-20}	4.9×10^{-19}
Ag_{18}	1.7×10^{-14}	29	5.1×10^{-19}	1	5.1×10^{-19}	1.7×10^{-14}
Ag_{19}	3.7×10^{-13}	9.0×10^{-2}	1.1×10^{-17}	1	1.1×10^{-17}	1.1×10^{-18}
Ag_{20}	4.4×10^{-15}	1.5	1.3×10^{-19}	1	1.3×10^{-19}	2.0×10^{-19}
Ag_{25}	3.8×10^{-11}	2.0×10^{-2}	1.1×10^{-15}	1	1.1×10^{-15}	2.3×10^{-17}
Ag_{26}	4.5×10^{-14}	11	1.3×10^{-18}	1	1.3×10^{-18}	1.5×10^{-17}
			$Ag_{n-1}Ir$			
Ag_2Ir	2.6×10^{7}	3.5×10^{6}	1.00	0.0013	0.013	4.4×10^{3}
Ag_3Ir	3.7×10^{4}	5.8×10^{5}	0.52	0.47	0.24	1.4×10^{5}
Ag_4Ir	7.7	4.0×10^{8}	2.3×10^{-4}	1	2.3×10^{-4}	9.3×10^{4}
Ag_5Ir	2.1×10^{5}	1.4×10^{7}	0.86	0.17	0.15	1.6×10^{6}
Ag_6Ir	1.6×10^{-3}	2.1×10^{8}	4.8×10^{-8}	1	4.8×10^{-8}	10
Ag_7Ir	7.7	5.5×10^{6}	2.3×10^{-4}	1	2.3×10^{-4}	1.3×10^{3}
Ag_8Ir	1.9×10^{-4}	3.6×10^{9}	5.8×10^{-9}	1	5.8×10^{-9}	21
Ag_9Ir	1.5×10^{-12}	7.0×10^{8}	4.4×10^{-17}	1	4.4×10^{-17}	3.1×10^{-8}
$Ag_{10}Ir$	1.9×10^{-5}	3.6×10^{-4}	5.7×10^{-10}	1	5.7×10^{-10}	2.1×10^{-13}
$Ag_{13}Ir$	4.7×10^{-10}	7.0	1.4×10^{-14}	1	1.4×10^{-14}	9.9×10^{-14}
$Ag_{17}Ir$	4.6×10^{-12}	0.57	1.4×10^{-16}	1	1.4×10^{-16}	8.0×10^{-17}

$Ag_{18}Ir$	4.7×10^{-10}	7.6×10^{-5}	1.4×10^{-14}	1	1.4×10^{-14}	1.1×10^{-18}
$Ag_{19}Ir$	3.1×10^{-12}	1.2	9.4×10^{-17}	1	9.4×10^{-17}	1.1×10^{-16}
$Ag_{24}Ir$	6.9×10^{-10}	1.9	2.1×10^{-14}	1	2.1×10^{-14}	3.9×10^{-14}
$Ag_{25}Ir$	3.8×10^{-13}	1.8×10^{2}	1.1×10^{-17}	1	1.1×10^{-17}	2.0×10^{-15}

TableS11. K and k (s^{-1}) are the equilibrium constant and O_2 direct dissociation rate constant, respectively. θ_{O2} and θ^* are the coverages of O_2 and free sites of the clusters. r (molecules$\cdot s^{-1}\cdot site^{-1}$) stand for the reaction rate for O_2 direct dissociation process at T=600 K and $P_{O2}=3\times10^{-4}$Pa.

Ag_n						
Clusters	K	k	θ_{O_2}	θ_*	$\theta_{O_2} * \theta_*$	r
Ag_3	4.0×10^{-6}	1.5×10^{-7}	1.2×10^{-9}	1	1.2×10^{-9}	1.8×10^{-16}
Ag_4	2.1×10^{-12}	4.4×10^{-4}	6.4×10^{-16}	1	6.4×10^{-16}	2.8×10^{-19}
Ag_5	8.5×10^{-8}	3.4×10^{-7}	2.6×10^{-11}	1	2.6×10^{-11}	8.8×10^{-18}
Ag_6	1.4×10^{-14}	7.0×10^{-7}	4.2×10^{-18}	1	4.2×10^{-18}	2.9×10^{-24}
Ag_7	1.8×10^{-9}	7.6×10^{-4}	5.4×10^{-13}	1	5.4×10^{-13}	4.1×10^{-16}
Ag_8	2.1×10^{-14}	9.9×10^{-5}	6.2×10^{-18}	1	6.2×10^{-18}	6.2×10^{-22}
Ag_9	1.8×10^{-8}	3.4	5.5×10^{-12}	1	5.5×10^{-12}	1.9×10^{-11}
Ag_{10}	3.1×10^{-11}	0.60	9.4×10^{-15}	1	9.4×10^{-15}	5.7×10^{-15}
Ag_{11}	2.6×10^{-10}	3.8×10^{-9}	7.9×10^{-14}	1	7.9×10^{-14}	3.0×10^{-22}
Ag_{14}	1.4×10^{-15}	12	4.2×10^{-19}	1	4.2×10^{-19}	4.9×10^{-18}
Ag_{18}	1.7×10^{-14}	29	5.1×10^{-18}	1	5.1×10^{-18}	1.5×10^{-16}
Ag_{19}	3.7×10^{-13}	9.0×10^{-2}	1.1×10^{-16}	1	1.1×10^{-16}	1.1×10^{-17}
Ag_{20}	4.4×10^{-15}	1.5	1.3×10^{-18}	1	1.3×10^{-18}	2.0×10^{-18}
Ag_{25}	3.8×10^{-11}	2.0×10^{-2}	1.1×10^{-14}	1	1.1×10^{-14}	2.3×10^{-16}
Ag_{26}	4.5×10^{-14}	11	1.3×10^{-17}	1	1.3×10^{-17}	1.5×10^{-16}
			$Ag_{n-1}Ir$			
Ag_2Ir	2.6×10^{7}	3.5×10^{6}	1.00	0.00013	0.00013	4.4×10^{3}
Ag_3Ir	3.7×10^{4}	5.8×10^{5}	0.92	0.082	0.076	1.4×10^{5}
Ag_4Ir	7.7	4.0×10^{8}	2.3×10^{-3}	1	2.3×10^{-3}	9.3×10^{4}
Ag_5Ir	2.1×10^{5}	1.4×10^{7}	0.98	0.016	0.015	1.6×10^{6}
Ag_6Ir	1.6×10^{-3}	2.1×10^{8}	4.8×10^{-7}	1	4.8×10^{-7}	10
Ag_7Ir	7.7	5.5×10^{6}	2.3×10^{-4}	1	2.3×10^{-3}	1.3×10^{3}
Ag_8Ir	1.9×10^{-4}	3.6×10^{9}	5.8×10^{-8}	1	5.8×10^{-8}	21
Ag_9Ir	1.5×10^{-12}	7.0×10^{8}	4.4×10^{-16}	1	4.4×10^{-16}	3.1×10^{-8}
$Ag_{10}Ir$	1.9×10^{-5}	3.6×10^{-4}	5.7×10^{-9}	1	5.7×10^{-9}	2.1×10^{-13}
$Ag_{13}Ir$	4.7×10^{-10}	7.0	1.4×10^{-13}	1	1.4×10^{-13}	9.9×10^{-14}
$Ag_{17}Ir$	4.6×10^{-12}	0.57	1.4×10^{-15}	1	1.4×10^{-15}	8.0×10^{-17}
$Ag_{18}Ir$	4.7×10^{-10}	7.6×10^{-5}	1.4×10^{-13}	1	1.4×10^{-13}	1.1×10^{-18}

$Ag_{19}Ir$	3.1×10^{-12}	1.2	9.4×10^{-16}	1	9.4×10^{-16}	1.1×10^{-16}
$Ag_{24}Ir$	6.9×10^{-10}	1.9	2.1×10^{-13}	1	2.1×10^{-13}	3.9×10^{-14}
$Ag_{25}Ir$	3.8×10^{-13}	1.8×10^{2}	1.1×10^{-16}	1	1.1×10^{-16}	2.0×10^{-15}

TableS12. The bond length, coordination numbers (CN), E^{mon}, E^{dim}, O_2 adsorption energy (E_{ads}) of Ag_{10}, Ag_8Ir for PBE and TPSS functional.

Ag_{10}	PBE	TPSS	Ag_8Ir	PBE	TPSS
R(Ag-Ag) /Å	2.83	2.77	R(Ag-Ag)/Å	2.92	2.85
-	-	-	R(Ag-Ir)/Å	2.68	2.65
CN(Ag-Ag)	4.80	4.80	CN(Ag-Ag)	3.75	3.75
-	-	-	CN(Ag-Ir)	1	1
E^{mon} /(eV)	2.11	2.27	E^{mon}/(eV)	2.53	2.83
E^{dim} /(eV)	1.63	1.87	E^{dim}/(eV)	2.87	3.22
E_{ads} /(eV)	0.57	0.38	E_{ads}/(eV)	1.38	1.45

Fig. S1 : Total densities of states of two typical clusters : Ag_6 (left) and Ag_5Ir (right)clusters.