Supporting Materials for

Vacancy Formation Energy as an Effective Descriptor for the Catalytic Oxidation of CO by Au Nanoparticles

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Table S1. The molecular dynamics simulation data and calculation results of Au nanoparticles.

R	1.97	2.21	2.47	2.75	3.01	3.25	3.51	3.77	4.04	4.31
r_0	0.1442	0.1442	0.1442	0.1442	0.1442	0.1442	0.1442	0.1442	0.1442	0.1442
N	1887	2664	3719	5133	6730	8515	10722	13281	16339	19834
N_0	2048	2916	4000	5324	6912	8788	10976	13500	16384	19652
$\dfrac{N_0 - N}{N_0}$	0.079	0.086	0.070	0.036	0.026	0.036	0.028	0.020	0.007	-0.005
$\dfrac{N_0 r_0^3}{\eta R^3}$	1.085	1.095	1.076	1.037	1.027	1.037	1.028	1.021	1.007	0.995

Table S2. The simulation data of Au nanoparticles.

	1	2	3	4	5	6	7	8	9
R (nm)	0.97	2.53	5.05	7.58	10.20	15.15	24.95	40.00	49.91
$E_v(R)/E_v(b)$	0.49	0.77	0.88	0.92	0.94	0.96	0.98	0.99	0.99

Table S3. The simulation data of Au nanoparticles.

	1	2	3	4	5	6	7	8	9	10
R (nm)	6.12	10.97	16.02	20.88	26.02	30.97	36.02	41.17	45.92	2.18
$E_v(r)/E_v$	0.90	0.94	0.96	0.97	0.98	0.98	0.98	0.99	0.99	0.72

Table S4. The simulation data of Au nanoparticles.

	1	2	3	4	5	6	7	8	9	10
R (nm)	0.97	6.02	11.17	15.92	20.97	26.22	30.97	35.92	40.97	46.02
$E_v(r)/E_v$	0.72	0.94	0.97	0.98	0.98	0.99	0.99	1.00	1.00	1.00

Table S5. The calculation parameter of the vacancy formation energy of Au nanoparticles.

Structure	r_{Au}	CN	ρ_r/ρ_0	η	U_m (kJ mol^{-1})	E_v (eV)	T_m (K)	Q_m (eV/atom)
FCC	0.1442	12	0.9	0.74	368	1.03	1337	2.1

Table S6. The size effect of the vacancy formation energy of Au nanoparticles' (111) crystal surface.

	1	2	3	4	5	6	7	8	9	10
R (nm)	1.10	1.15	1.20	1.25	1.30	1.50	1.50	1.60	1.60	1.77
$E_v(R\text{-}111)/E_v(111)$	0.14	0.14	0.14	0.15	0.15	0.18	0.16	0.17	0.15	0.20
	11	12	13	14	15	16	17	18	19	20
R (nm)	1.80	1.91	1.90	2.00	2.00	2.00	2.10	2.15	2.40	3.00
$E_v(R\text{-}111)/E_v(111)$	0.24	0.21	0.15	0.15	0.16	0.18	0.16	0.16	0.17	0.16
	21	22	23	24	25	26	27	28	29	30
R (nm)	3.50	4.00	6.50	7.95	11.00	13.08	19.09	22.86	20.06	17.15
$E_v(R\text{-}111)/E_v(111)$	0.21	0.24	0.22	0.25	0.22	0.22	0.21	0.21	0.25	0.24

Table S7. The size effect of the vacancy formation energy of Ag nanoparticles' (111) crystal surface.

	1	2	3	4	5	6	7	8	9	10
R (nm)	1.25	1.40	1.75	1.95	2.19	2.30	2.37	2.40	2.47	2.50
$E_v(R\text{-}111)/E_v(111)$	0.12	0.12	0.13	0.14	0.14	0.15	0.14	0.16	0.15	0.15
	11	12	13	14	15	16	17	18	19	20
R (nm)	2.70	2.85	3.05	3.35	3.20	3.30	3.50	3.68	4.18	4.38
$E_v(R\text{-}111)/E_v(111)$	0.14	0.17	0.18	0.16	0.19	0.19	0.23	0.19	0.19	0.25
	21	22	23	24	25	26	27	28	29	30
R (nm)	4.45	4.78	4.38	5.38	7.80	9.18	3.41	--	--	--
$E_v(R\text{-}111)/E_v(111)$	0.22	0.20	0.20	0.23	0.25	0.25	0.27	--	--	--

Table S8. The size effect of the vacancy formation energy of Cu nanoparticles' (111) crystal surface.

	1	2	3	4	5	6	7	8	9	10

R (nm)	1.20	1.20	1.50	1.51	1.50	2.22	2.50	2.50	3.38	3.70
$E_v(R\text{-}111)/E_v(111)$	0.14	0.15	0.13	0.16	0.17	0.17	0.13	0.17	0.20	0.17
	11	12	13	14	15	16	17	18	19	20
R (nm)	3.71	4.00	5.00	5.5	5.95	7.01	7.94	9.08	--	--
$E_v(R\text{-}111)/E_v(111)$	0.20	0.19	0.20	0.18	0.18	0.21	0.21	0.22	--	--

Table S9. The calculation parameter of the vacancy formation energy of Au, Ag, and Cu nanoparticles' (111) crystal surfaces.

Au	Structure	r_{Au}	CN	ρ_r/ρ_0	η	k
	FCC	0.1442	9	0.9	0.74	0.25
Ag	Structure	r_{Au}	CN	ρ_r/ρ_0	η	k
	FCC	0.144	9	0.9	0.74	0.25
Cu	Structure	r_{Au}	CN	ρ_r/ρ_0	η	k
	FCC	0.128	9	0.9	0.74	0.25

Table S10. The constant pressure heat capacity (C_p (J·mol^{-1}K) simulation data of Au nanoparticles.

LH	1	2	3	4	5	6	7	8	9	10
T (K)	100.00	200.00	300.00	400.00	500.00	600.00	700.00	800.00	900.00	1000.00
$E_v(R,T)/E_v$	0.99	0.98	0.97	0.97	0.97	0.97	0.97	0.96	0.96	0.95

ELH	1	2	--	QH	1	2	--	--	--	--
T (K)	200..00	800.00	--	T (K)	200.00	800.00	--	--	--	--
$E_v(R,T)/E_v$	0.98	0.94	--	$E_v(R)/E_v$	0.98	0.93	--	--	--	--

Table S11. The calculation parameter of the constant pressure heat capacity (C_p (J·mol^{-1}K) of Au nanoparticles.

	1	2	3	4	5	6	7	8	9	10	11
T	273.15	298.15	373.15	473.15	573.15	673.15	773.15	873.15	900.00	900.000	1073.15
C_p J·mol^{-1}K	25.21	25.29	25.59	26.031	26.479	26.92	27.34	27.74	27.85	27.83	29.00

Table S12. The simulation data from Li's model of Au nanoparticles.

0 K	1	2	3	4	5	6	7	8	9
R (nm)	1.00	2.50	5.00	7.50	10.00	15.00	25.00	40.00	50.00
$E_v(R)/E_v$	0.51	0.80	0.91	0.95	0.97	0.99	1.00	1.01	1.03
300 K	10	11	12	13	14	15	16	17	18
R (nm)	1.00	2.50	5.00	7.50	10.00	15.00	25.00	40.00	50.00
$E_v(R)/E_v$	0.50	0.78	0.89	0.93	0.95	0.97	0.99	1.00	1.02
800 K	10	20	21	22	23	24	25	26	27
R (nm)	1.00	2.50	5.00	7.50	10.00	15.00	25.00	40.00	50.00
$E_v(R)/E_v$	0.48	0.75	0.86	0.90	0.92	0.94	0.95	0.96	0.97
Melting K	28	29	30	31	32	33	34	35	36
R (nm)	1.00	2.50	5.00	7.50	10.00	15.00	25.00	40.00	50.00
$E_v(R)/E_v$	0.46	0.72	0.82	0.86	0.88	0.89	0.91	0.92	0.92

Table S13. The simulation data from Ouyang's model of Au nanoparticles in 0 K.

0 K	1	2	3	4	5	6	7	8	9
R (nm)	0.69	1.00	1.31	1.92	3.62	5.92	8.23	10.54	12.85
$E_v(R)/E_v$	0.08	0.39	0.53	0.69	0.84	0.91	0.94	0.95	0.96
10	11	12	13	14	15	16	17	18	19
7.58	15.15	17.46	19.77	22.08	24.38	26.69	29.00	31.31	33.69
0.97	0.97	0.97	0.98	0.98	0.98	0.99	0.99	0.99	0.99
20	21	22	23	24	25	26	27	28	29
19.12	36.00	38.23	40.54	42.92	45.15	47.46	49.77	--	--

| 0.99 | 0.99 | 0.99 | 0.99 | 0.99 | 0.99 | 0.99 | 0.99 | -- | -- |

Table S14. The simulation data from Ouyang's model of Au nanoparticles in 300 K.

300 K	1	2	3	4	5	6	7	8	9
R (nm)	1.28	1.51	3.56	5.86	8.16	10.47	12.77	15.07	17.38
E_v®/E_v	0.33	0.40	0.62	0.68	0.70	0.72	0.73	0.73	0.74
10	**11**	**12**	**13**	**14**	**15**	**16**	**17**	**18**	**19**
19.68	22.00	24.29	26.59	28.90	31.20	33.51	35.81	38.11	40.42
0.74	0.74	0.74	0.74	0.74	0.75	0.75	0.75	0.75	0.75
20	**21**	**22**	**23**	**24**	**25**	**26**	**27**	**28**	**29**
42.72	45.03	47.33	49.63	--	--	--	--	--	--
0.75	0.75	0.75	0.75	--	--	--	--	--	--

Table S15. The Linear relationship between the chemical bond energy and vacancy formation of face-centered cubic crystals.

Elements	W	Ta	Mo	Zr	Pt	V	Ti	Co	Cr
E_m (kJmol^{-1})	838.62	784.71	660.42	612.60	564.71	510.88	489.89	427.07	395.64
E_v (eV)	2.21	2.01	1.55	1.53	1.40	1.32	1.21	1.10	1.00
Elements	**Fe**	**Au**	**Be**	**Al**	**Ag**	**Pb**	**Mg**	**Li**	**Zn**
E_m (kJmol^{-1})	416.57	367.24	320.85	322.32	286.39	198.12	160.69	147.25	129.27
E_v (eV)	1.03	0.98	0.86	0.83	0.70	0.51	0.37	0.38	0.30

Table S16. Linear relationship between vacancy-forming energy and diffusion activation energy in common metal materials.

	Al	Cd	Co	Cu	Au	Fe	Pb	Li	Pt	Ag	Na	W	Zn
E_v (eV)	0.84	0.29	1.1	0.88	0.98	1.03	0.51	0.38	1.4	0.23	0.71	0.28	0.34
Q(eV)	1.43	0.81	2.9	2.04	1.7	3.17	1.05	0.41	2.5	0.39	1.91	0.45	1