Supplementary Materials: A Theoretical Insight into Enhanced Catalytic Activity of Au by Multiple Twin Nanoparticles

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Table S1. List of calculated adsorption energies. S_z is the z component of spin. CN is coordination number of adsorption site. Avg. RMSD is the average value of root-mean-square distances (RMSDs) of NP atoms before and after CO adsorption.

Adsorption Site	Symmetry	S_z	CN	Number of Au atoms of NP	E_{ad} /eV	Average surface CN	Ratio of surface atoms	Avg. RMSD /pm
Vertex[*1]	D_{5h}	0	6	54	−0.76	7.1	0.87	–––
	D_{5h}	1/2	6	49	−0.84	7.0	0.86	–––
Vertex	D_{5h}	0	6	54	−1.03	7.1	0.87	13.9
	D_{5h}	0	6	100	−0.84	7.4	0.77	4.6
	D_{5h}	0	6	176	−0.80	7.6	0.69	1.8
	D_{5h}	0	6	282	−0.78	8.0	0.63	1.2
	O_h	1/2	5	55	−0.87	6.6	0.76	3.1
	O_h	1/2	5	147	−0.88	7.2	0.63	1.3
	O_h	1/2	5	309	−0.91	7.5	0.52	1.1
	D_{5h}	1/2	6	49	−0.96	7.0	0.86	7.2
	D_{5h}	1/2	6	105	−0.82	7.5	0.78	2.1
	D_{5h}	1/2	6	181	−0.75	7.6	0.70	1.7
	D_{5h}	1/2	6	287	−0.75	8.0	0.63	1.3
Vertex (GB)	D_{3h}	1/2	5	55	−0.85	6.6	0.76	2.8
	D_{3h}	1/2	5	147	−0.86	7.2	0.63	2.1
	D_{3h}	1/2	5	309	−0.88	7.5	0.52	1.3
Edge	O_h	1/2	7	55	−0.64	6.6	0.76	4.5
	O_h	1/2	7	147	−0.64	7.2	0.63	2.7
	O_h	1/2	7	309	−0.64	7.5	0.52	2.3
	D_{5h}	1/2	8	49	−0.67	7.0	0.86	8.1
	D_{5h}	1/2	8	181	−0.39	7.6	0.70	2.7
	D_{5h}	1/2	8	287	−0.41	8.0	0.63	2.5
(100) face	O_h	1/2	8	55	−0.70	6.6	0.76	5.0
	O_h	1/2	8	147	−0.40	7.2	0.63	3.4
	O_h	1/2	8	309	−0.54	7.5	0.52	2.4

(111) face	O_h	1/2	9	147	−0.37	7.2	0.63	3.6
	O_h	1/2	9	309	−0.35	7.5	0.52	1.6
	D_{5h}	1/2	9	49	−0.90	7.0	0.86	26.4
	D_{5h}	1/2	9	181	−0.19	7.6	0.70	4.1
	D_{5h}	1/2	9	287	−0.19	8.0	0.63	2.7

*1 Optimization of adsorption structure with fixing the geometry of NPs.