

Supporting Information for
“Understanding the Effects of Au Morphology on
CO₂ Electrocatalysis”

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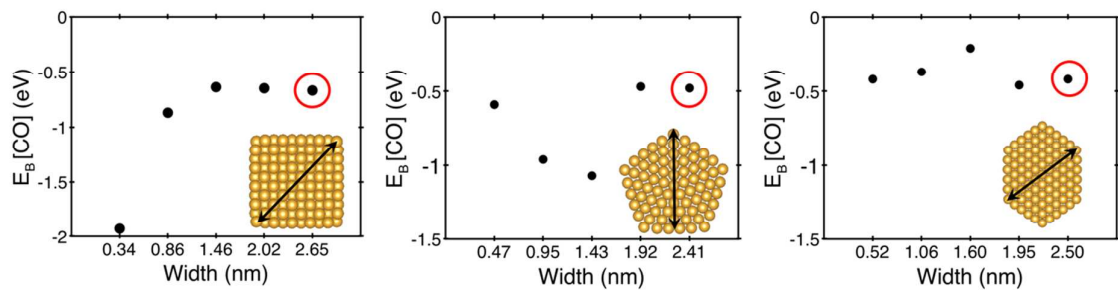


Figure S1. Binding energies of *CO ($E_B[*CO]$) at the edge sites of NW with various sizes.

NWs marked with red circles were used for further calculations.

Table S1. A summary of the usual coordination number (cn), the generalized coordination number (\overline{CN}), calculated $E_B[*H]$, $E_B[*CO]$ and $E_B[*COOH]$. Values in parenthesis correspond to *H binding cases, where cn and \overline{CN} for *H binding are, in some cases, different from those for *CO and *COOH binding, since the binding sites are different (bridge or hollow site for *H, and top site for *CO and *COOH). For the corner sites of cubo-NP and ico-NP, *H binding at the bridge sites between corner and adjacent atoms is more stable than atop binding on the corner atom.

	Models	cn	\overline{CN}	$E_B[*CO]$	$E_B[*COOH]$	$E_B[*H]$
Edge Sites	s-NW	5.00	3.67 (4)	-0.67	1.28	0.13
	p-NW	6.00	4.33 (4.44)	-0.48	1.26	0.12
	h-NW1	7.00	5.17 (5.11)	-0.41	1.45	0.19
	h-NW2	7.00	5.33 (5.17)	-0.42	1.29	0.11
	ico-NP	8.00	6.33 (5.67)	-0.38	1.53	0.13
	cubo-NP	7.00	5.33 (4.94)	-0.48	1.47	-0.05
	cubic-NP	5.00	3.67 (4)	-0.69	1.25	0.09
Corner Sites	ico-NP	6.00 (7.00)	4.33 (4.56)	-0.52	1.33	0.18
	cubo-NP	5.00 (6.00)	3.33 (3.83)	-0.78	1.09	-0.05
	cubic-NP	3.00	2.00	-0.80	1.12	0.07
Facets	Au (111)	9.00	7.50 (6.95)	0.00	1.84	0.28
	Au (100)	8.00	6.67	-0.31	1.60	0.13
	Au (110)	7.00	5.83 (5.78)	-0.40	1.45	0.17
	Au (211)	7.00	5.50 (5.39)	-0.46	1.46	0.08

Table S2. The number and the density of edge and corner sites of the models shown in **Figure 5.**

	Models	Edge sites	Corner sites
A	8 nm ico-NP (10,179 atoms)	$13 \times 30 = 390$ (3.83 %)	12 (0.12 %)
B	4 nm ico-NP (11,320 atoms) (8 × 1415 atom NP)	$8 \times 6 \times 30 = 1,440$ (12.72 %)	$8 \times 12 = 96$ (0.85 %)
C	2 nm p-NW (10,140 atoms)	(NW edges) (NW caps) $192 \times 5 + 30 \times 2 = 1,020$ (10.06%)	$6 \times 2 = 12$ (0.12 %)