Supporting Information

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The Effect of Pd Nanoparticle Size on the Catalytic Hydrogenation of Allyl Alcohol

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(8 pages)

Table S1. Calculated and measured particle diameters and TOFs based on the number of moles of surface, defect, and face atoms and moles of DENs, for G6-OH(Pd_n) (n = 55, 100, 147, 200, 250) DENs.

n, G6-OH(Pd_n)	calculated diameter[a] (nm)	TEM diameter (nm)	$TOF^b_{surface}$	TOF^c_{defect}	TOF^d_{face}	TOF^e_{DENs}
55	1.2	1.3 ± 0.3	74 ± 1	87 ± 1	515 ± 5	31 ± 3
100	1.4	1.4 ± 0.3	86 ± 7	118 ± 10	353 ± 30	56 ± 5
147	1.6	1.5 ± 0.4	91 ± 2	139 ± 2	262 ± 5	85 ± 2
200	1.8	1.7 ± 0.3	107 ± 7	180 ± 9	270 ± 10	122 ± 6
250	1.9	1.9 ± 0.3	120 ± 6.0	218 ± 1	276 ± 2	163 ± 1

[a]calculated using the equation $n=4r^3/3V_g$ where n is the number of Pd atoms, r is the nanoparticle radius and V_g is the volume of one Pd atoms (15 $Å^3$)

[b]TOF = 10 mol H_2/(mol surface atoms-h)

[c]TOF = 10 mol H_2/(mol defect atoms-h)

[d]TOF = 10 mol H_2/(mol face atoms-h)

[e]TOF = 10^3 mol H_2/(mol nanoparticles-h)

Table S2. Formulae used to calculate m, the number of shells for nanoparticles having cuboctahedron geometry, and the number of Pd atoms at the various positions available on nanoparticle surfaces.[20] Two of the five nanoparticles examined in this study (G6-OH(Pd_n, n = 55 and 147) have complete outer shells with m = 3 and 4, respectively. The nanoparticles having n = 100, 200, and 250 have incomplete shells, with m = 3.56, 4.38, and 4.69 respectively.

Total no. atoms	$1/3(2m - 1)(5m^2 - 5m + 3)$
No. surface atoms	$10m^2 - 20m + 12$
Vertex atoms (5-coordinate)	12
Edge atoms (7-coordinate)	$24(m - 2)$
Sq. face (8-coordinate)	$6(m - 2)^2$
Triangular face (9-coordinate)	$4(m - 3)(m - 2)$

Table S3. Number of Pd atoms, and the corresponding number of moles (in italics), at each position on the surface of G6-OH(Pd_n) DENs, calculated using the formulae shown in Table S2.[20]

n, G6-OH(Pd_n)	surface atoms per particle *μmoles Pd*	defect atoms* per particle *μmoles Pd*	face atoms per particle *μmoles Pd*	DENs x 10^{15} *μmoles DENs*
55	42 *2.29*	36 *1.96*	6 *0.33*	33 *0.05*
100	67 *2.01*	49 *1.47*	18 *0.54*	18 *0.03*
147	92 *1.88*	60 *1.23*	32 *0.65*	12 *0.02*
200	116 *1.74*	69 *1.04*	47 *0.70*	9 *0.02*
250	138 *1.66*	76 *0.92*	62 *0.74*	7 *0.01*

*defect atoms = (vertex + edge) atoms

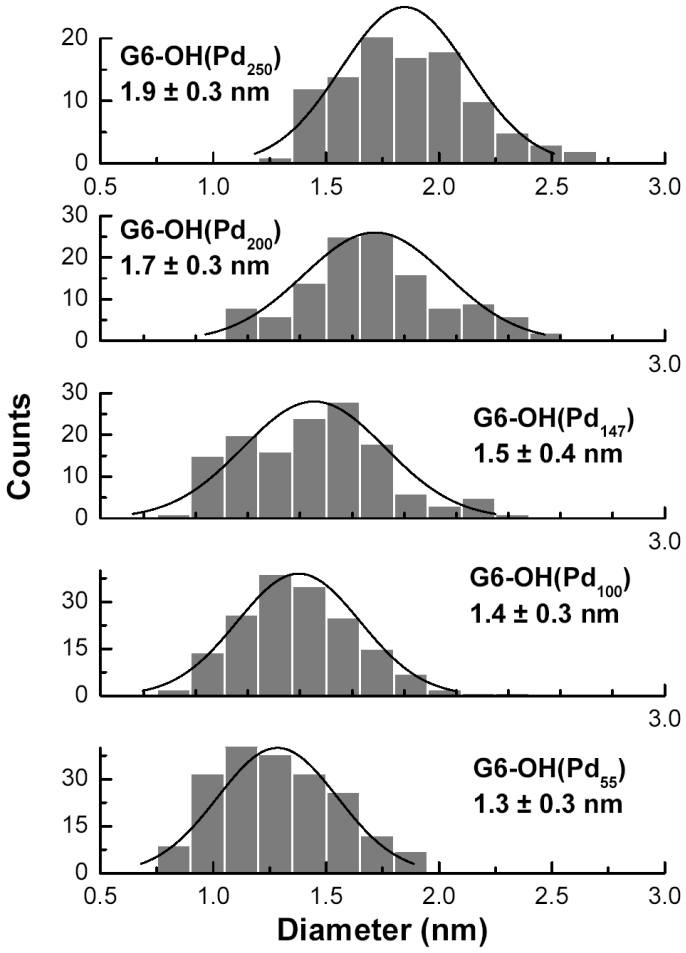

Figure S1. Particle-size histograms for G6-OH(Pd_n) (n = 55, 100, 147, 200, 250) DENs.

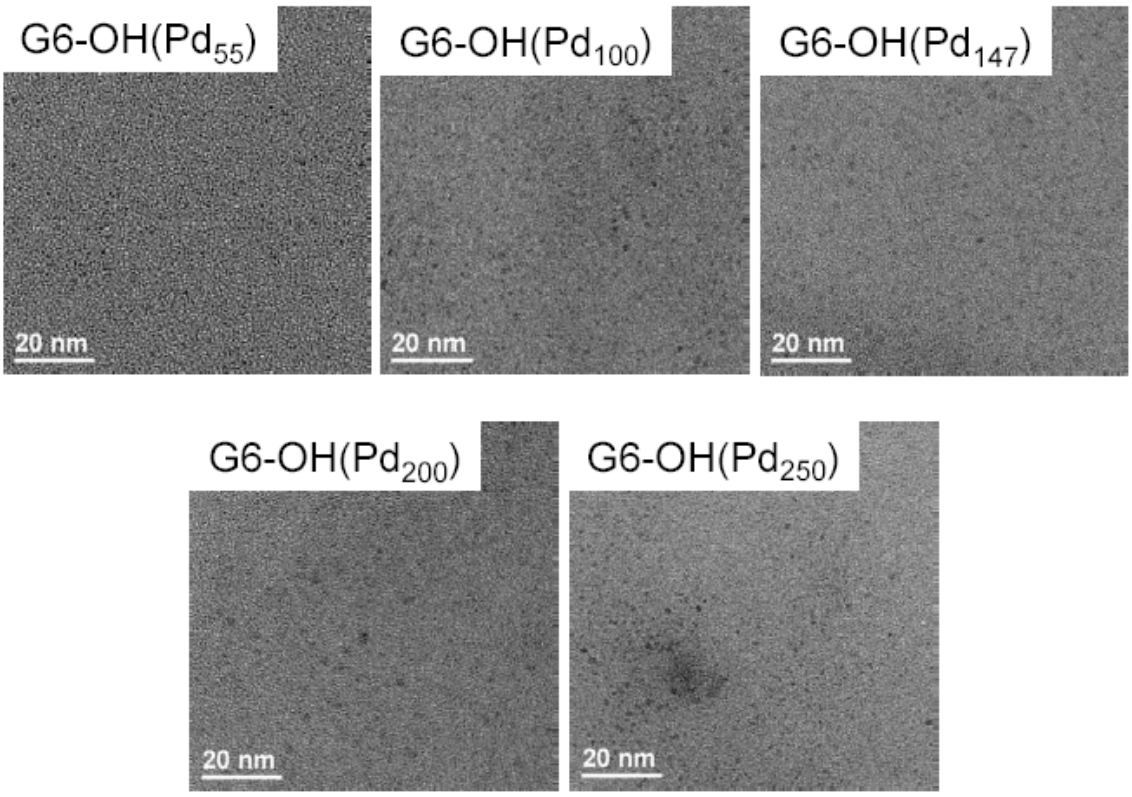

Figure S2. TEM micrographs of G6-OH(Pd_n) (n = 55, 100, 147, 200, 250) DENs.

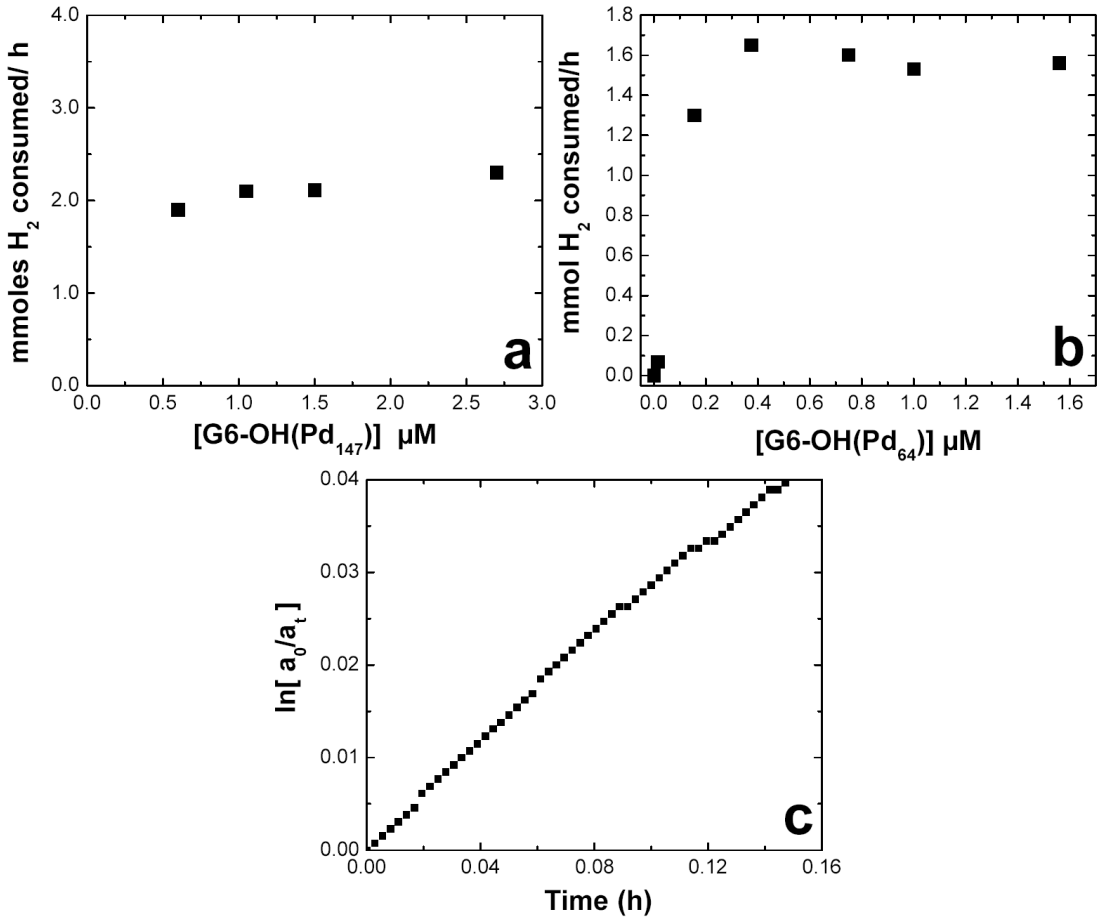

Figure S3. (a) Plot of reaction rate (mmol H_2 consumed/h) as a function of dendrimer concentration for G6-OH(Pd_{147}). (b) Plot of reaction rate (mmol H_2 consumed/h) as a function of dendrimer concentration for G6-OH(Pd_{64}). (c) Plot of $\ln[a_0/a_t]$ (where a_0 and a_t are the allyl alcohol concentrations at time = 0 and t, respectively) vs. time.

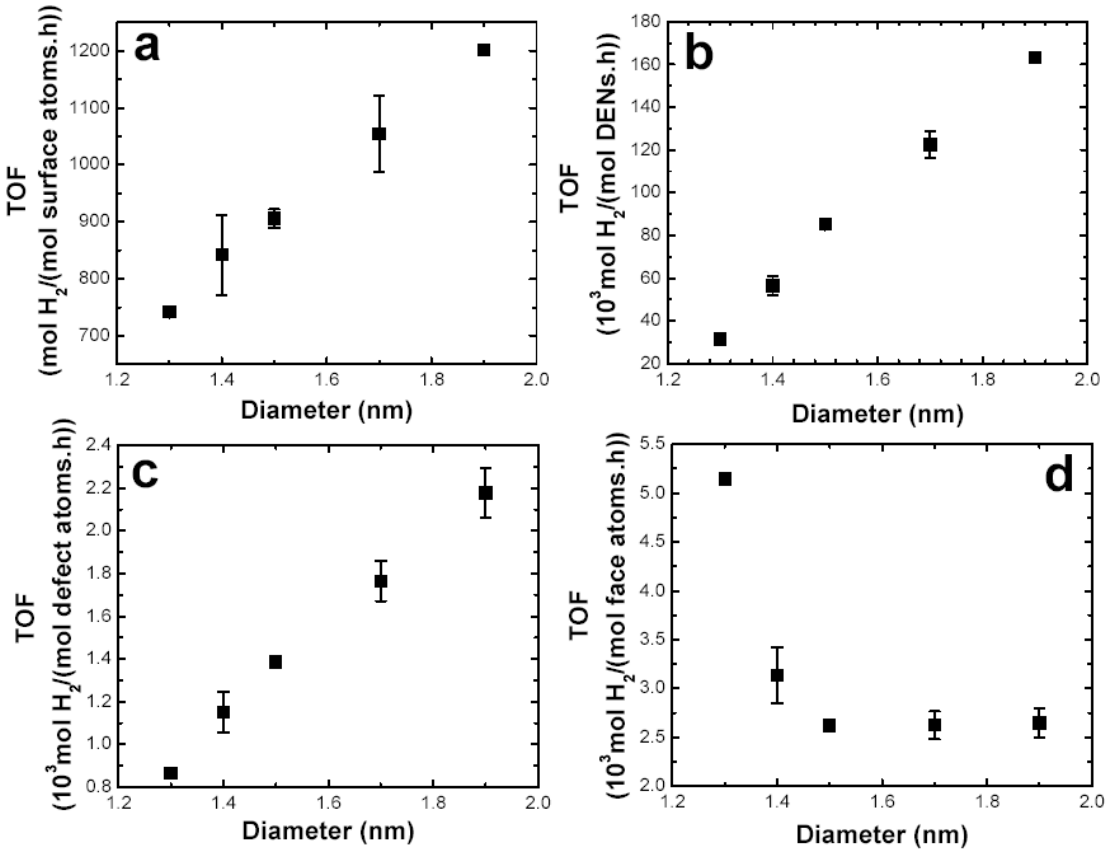

Figure S4. Plots of TOF as a function of particle diameter prior to normalization (the corresponding normalized data are provided in Figure 2). TOFs are calculated based on the number of moles of (a) surface atoms; (b) DENs; (c) defect atoms; and (d) face atoms.