Supporting Information

Determination of Nanoparticle Size by Measuring the Metal-Metal Bond Length: The Case of Palladium Hydride

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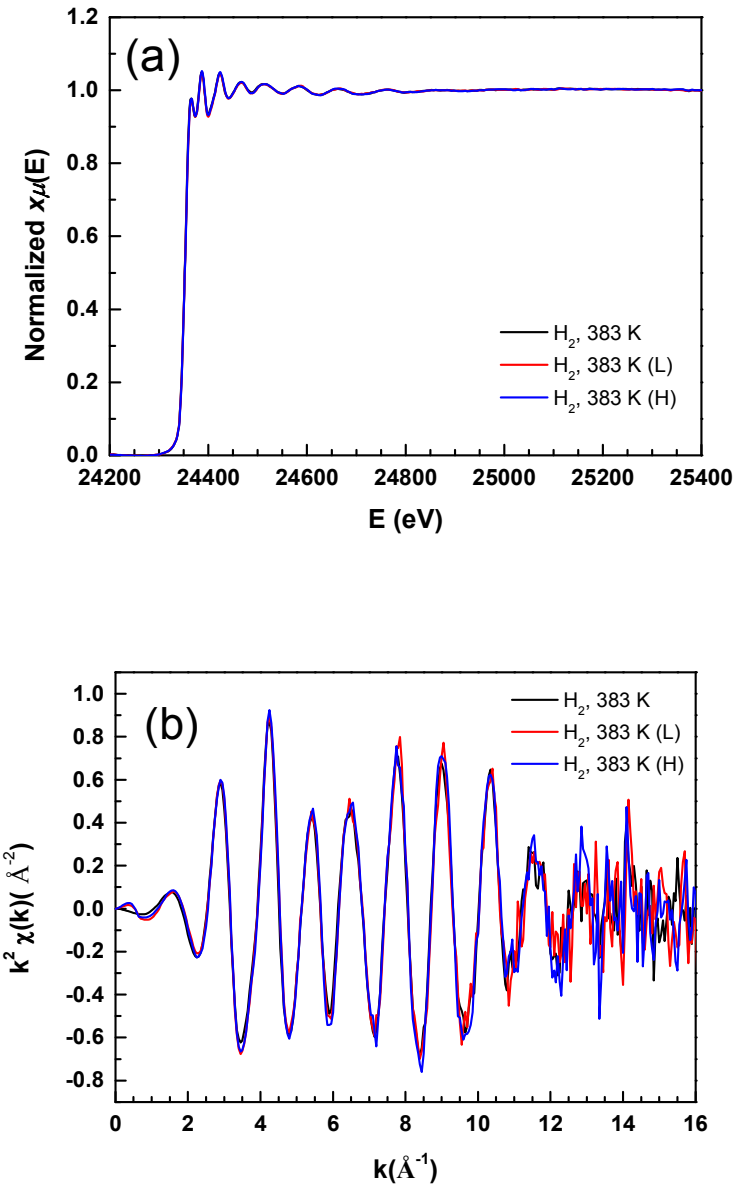

Figure S1. (a) Normalized XAS region of absorption coefficient of Pd K-edge. (b) EXAFS data of Pd catalyst under 50%H_2/He at same temperature (383 K). L stands for the data measured after reaching the lowest temperature of 186 K, and H stands for the one measured after reaching the highest temperature of 483 K. The temperature schedules are shown in Figure 1 of the manuscript.

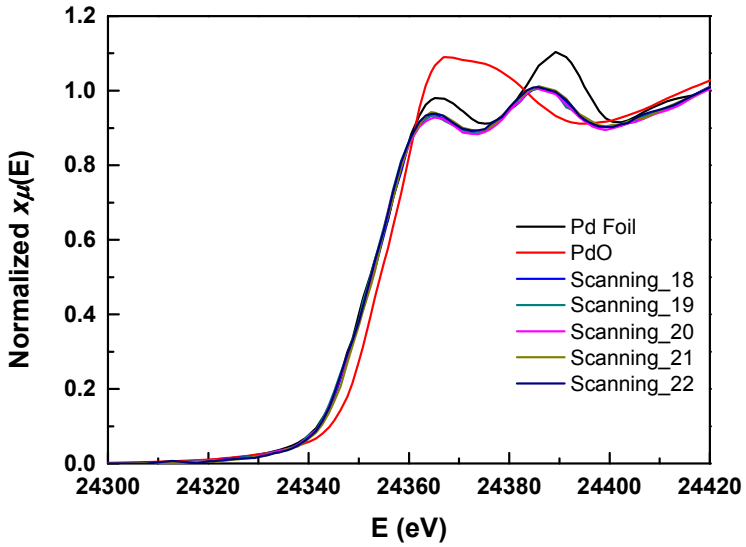

Figure S2. Normalized XANES region of absorption coefficient of Pd K-edge. Curves labeled Scanning_18 to Scanning_22 present the final 5 consecutive runs used for checking the stability of formation of reduced state.

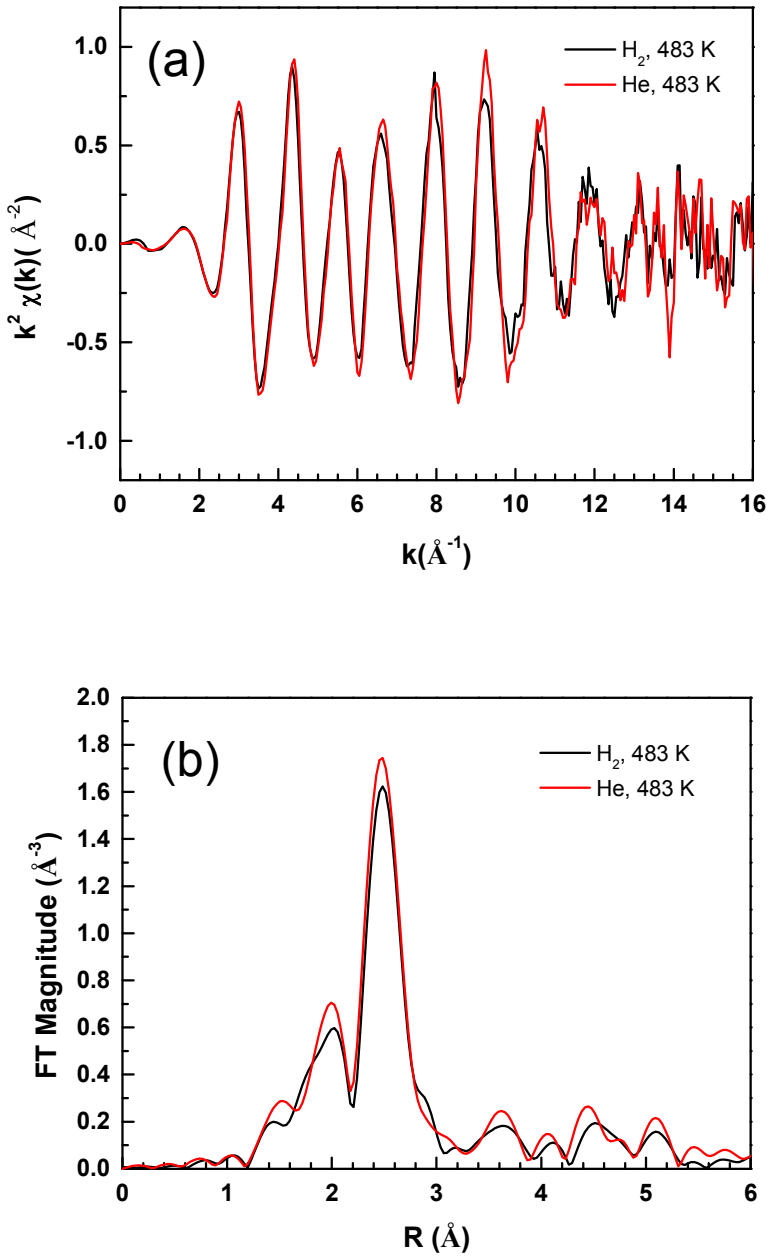

Figure S3. (a) EXAFS data measured under H_2 and He at 483 K in k-space (a) and r-space (b). k-weighting of 2 and k-range of 2-16 $Å^{-1}$ was used for Fourier transforms,

Table S1 The calculation of H/Pd ratio by a modified empirical equation[a]

Data	R (Å)	R_0 (Å)	δR	$\delta R/R_0$	x
H_2, 483 K	2.748(2)	-	0.015(4)	0.005(1)	0.08(2)
H_2, 383 K	2.799(3)	-	0.058(5)	0.021(2)	0.35(4)
H_2, 293 K	2.813(2)	-	0.072(3)	0.026(1)	0.44(2)
H_2, 186 K	2.826(1)	-	0.085(2)	0.031(1)	0.54(2)
He, 483 K	-	2.733(2)	-	-	-
He, 383 K	-	2.741(2)	-	-	-
He, 293 K	-	2.741(1)	-	-	-

[a]The modified empirical equation: $\frac{\delta R(T)}{R_0(T)} = 0.0666x - 0.0164x^2$, where *R(T)* is the bond length of Pd hydride at the temperature *T*; $R_0(T)$ is the bond length of bare metal particles free of hydrogen at the temperature of *T*; $\delta R(T)$ is defined as (R-R_0) and calculated at the same temperature; The value of R_0 for the data at 186 K is taken as 2.741(1) Å; x is the H/Pd ratio.