

Supporting Information:

Distinct Atomic Structure-Catalytic Activity Relationship in 3-10 nm Supported Au Particles

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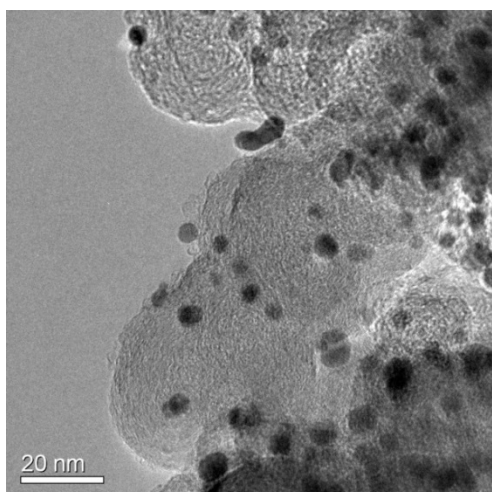
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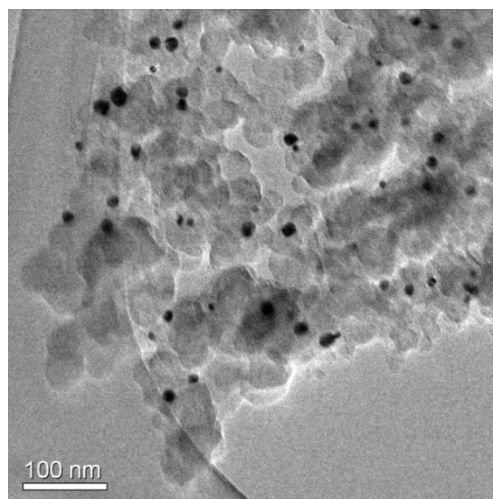
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Table S1. Comparison of the temperature at 50% conversion ($T_{1/2}$) for CO oxidation over silica and titania supported Au particles with sizes of 3 nm and 10 nm. The samples were "fresh" samples (O_2 - H_2 treated followed by air exposure), samples after O_2 -treatment only and samples after H_2 -treatment only.

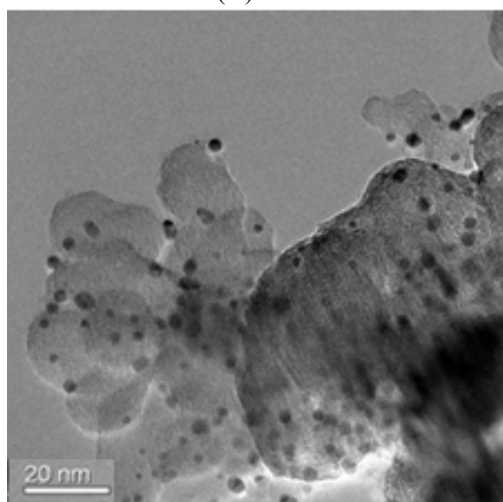
Au/Support	$T_{1/2}$ (°C)	
	Sample 3 nm	Sample 10 nm
<u>"Fresh" samples</u>		
/SiO ₂ (5% wt)	320	355
/TiO ₂ (5% wt)	260	265
<u>O₂ treated samples</u>		
/SiO ₂ (5% wt)	280	310
/TiO ₂ (5% wt)	210	120
<u>H₂ treated samples</u>		
/SiO ₂ (5% wt)	160	185
/TiO ₂ (5% wt)	80	50



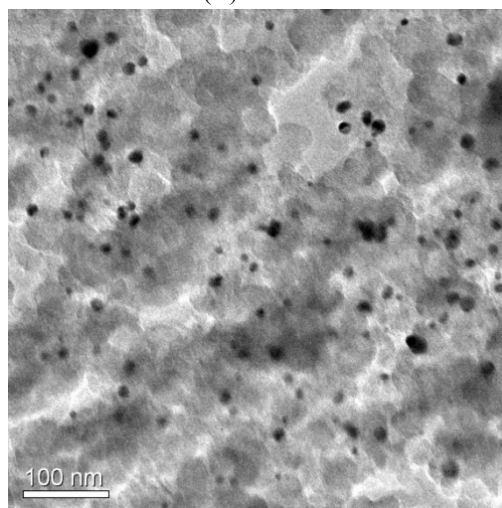
(A)



(B)



(C)



(D)

Figure S1. TEM images of $3.2 \text{ nm} \pm 1.0 \text{ nm}$ (A) and $10 \pm 1.7 \text{ nm}$ (B) Au/TiO₂ as well as of $3.4 \pm 1.0 \text{ nm}$ (C) and $10 \pm 1.9 \text{ nm}$ (D) Au/SiO₂ particles. Note the “ $\pm$ ” deviations from the average particles size are half widths at full maximum of the gaussian-like distribution of sizes extracted from populations of several hundreds of particles sampled by several TEM images.

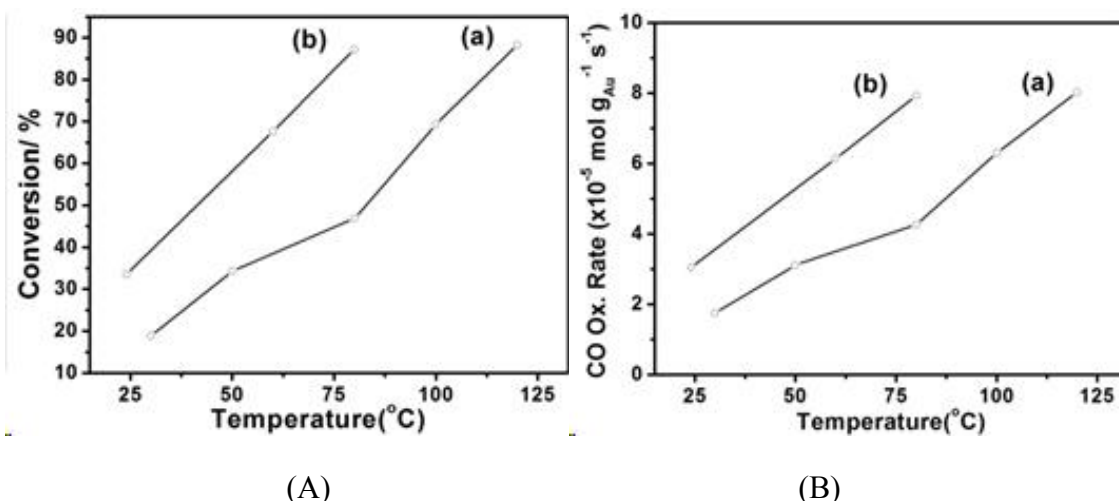


Figure S2. (A) CO conversion rate as a function of reaction temperature for titania supported Au particles with sizes of 3 nm (a) and 10 nm (b). The catalysts were treated under H₂ at 400 °C for 2 hrs before the measurement. (B) Au mass normalized conversion rate for the same catalysts.

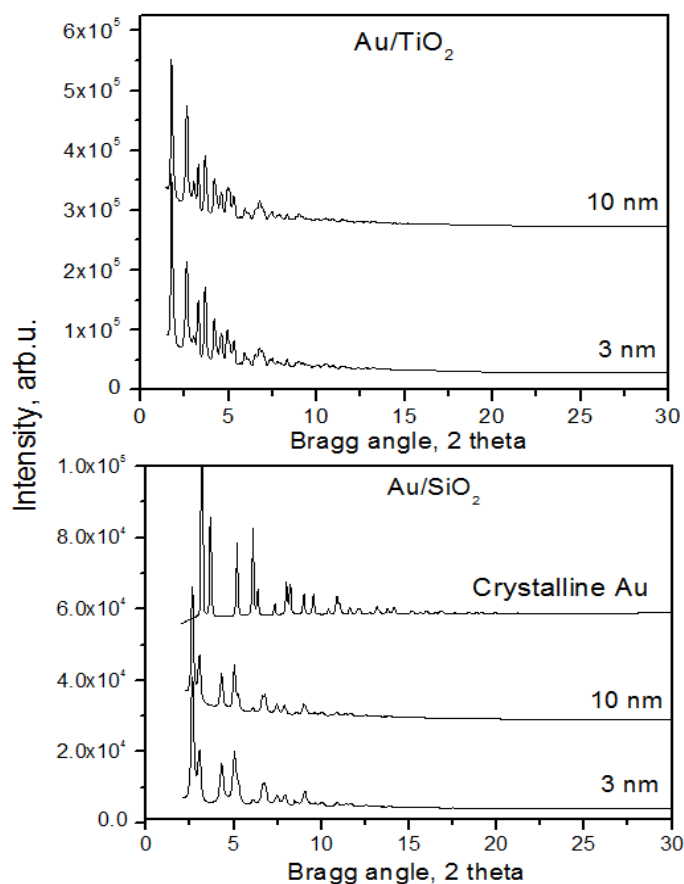


Figure S3: Experimental synchrotron x-ray diffraction patterns for Au NPs supported on silica and titania. The XRD pattern of polycrystalline Au standard is shown as well.

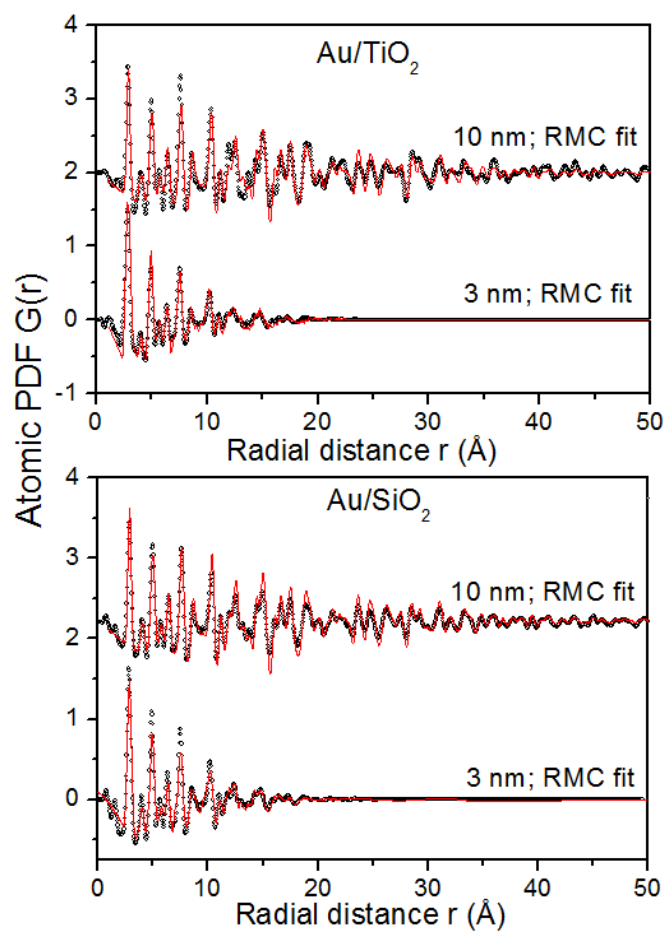


Figure S4: Experimental (symbols) and RMC model derived (line in red) atomic PDFs for Au NPs supported on titania and silica. The respective atomic configurations are shown in Fig. 5.