Supplemental Information for:

Identification of site requirements for reduction of 4-nitrophenol using gold nanoparticle catalysts

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Calculation of Reaction Rate Constant and Induction Time .........................2
Addition of additional 4-nitrophenol to reaction mixture after initial 4-nitrophenol is consumed .................................................................3
HAADF-STEM before and after reaction .........................................................4
Synthesis of gold nanoparticle catalysts .........................................................4
Calculation of Reaction Rate Constant and Induction Time

Pseudo-first order reaction rate constants were calculated by plotting ln(1-X) where X is the conversion of 4-NP versus time. The slope of the line of best fit in the plot gives the pseudo-first order rate constant. In some of the MBC samples, there were two negatively sloping regions, with one region having a significantly steeper slope. The most steeply sloped region was used to calculate the rate constant, and the less steep region was included as part of the induction time as shown in Fig. S1.

Figure S1: Kinetics plot of MBC-Au nanoparticle catalyzed reaction illustrating how the reaction rate was calculated and the induction time determined when there were two regions of different slope in the ln(1-X) versus time plots.
Addition of additional 4-nitrophenol to reaction mixture after initial 4-nitrophenol is consumed

Additional 4-NP was added to the reaction solution to achieve approximately the original concentration. The reaction proceeds without an induction time and the 4-NP begins to be consumed as it is added to the reaction mixture. Fig. S2 shows a plot of the relative concentration (referenced to the initial 4-NP concentration) as a function of time. The sharp peaks in the graph occurs after the doses of 4-NP are added to the reaction mixture. The fact that the value of $C/C_0 = 1$ is not observed after each addition can be explained by the fast reaction in the time in between when the 4-NP was added and the time until the first measurement taken after the addition.

![Graph](image)

Fig. S2: 4-NP concentration versus time of reaction plot using C6P-bound Au nanoparticles. No induction time is necessary upon adding the additional doses of 4-NP to the solution after the initial amount of 4-NP is consumed.
HAADF-STEM before and after reaction

TEM images were acquired before and after reaction and showed no significant particle morphology or size changes in solution as a result of the reaction. Fig. S3 shows the TEM images as well as the particle size histograms.

Fig. S3 (a) MBC-Au nanoparticles before reaction. (b) MBC-Au particles after reaction. The white scale bar represents 20 nm.

Synthesis of gold nanoparticle catalysts

Gold nanoparticle catalysts were synthesized according to literature procedures. (Refs 20-21 in manuscript). Prior to use in catalysis, the gold nanoparticles were exhaustively characterized using previously developed procedures, including accessibility measurements of 2-NT. These nanoparticles showed accessibility that was identical to values previously published in the literature (Refs. 20-21 in manuscript).