

Electronic Supplementary Information

Effect of Annealing in Oxygen on Alloy Structures of Pd–Au Bimetallic Model Catalysts

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1. AES Characterizations for Annealed Pd/Au(111) Surfaces

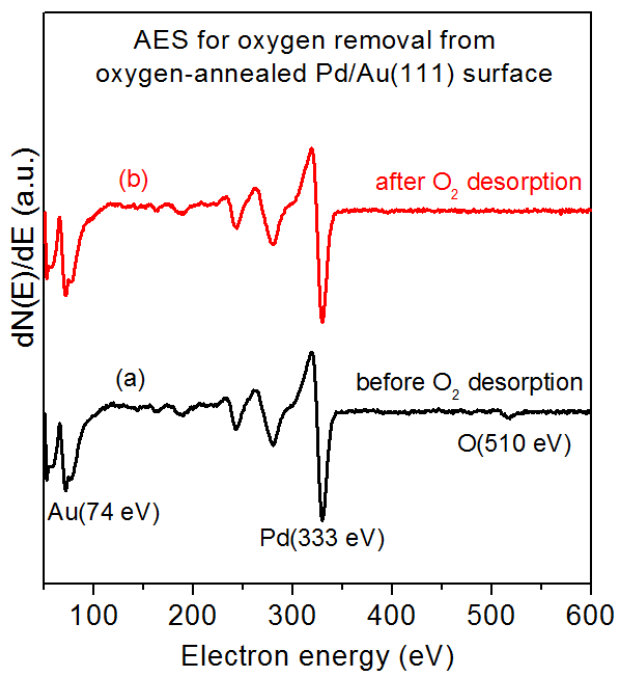


Figure S1. AES spectra of 1.5 ML Pd/Au(111) (a) immediately after annealing in 1×10^{-6} Torr of O₂ to 500 K for 10 min, and (b) after heating (a) surface to 500 K to desorb O₂.

2. Calculation of Initial Sticking Probability of O₂ on Annealed Pd/Au(111) Surface in O₂ King–Wells Measurement

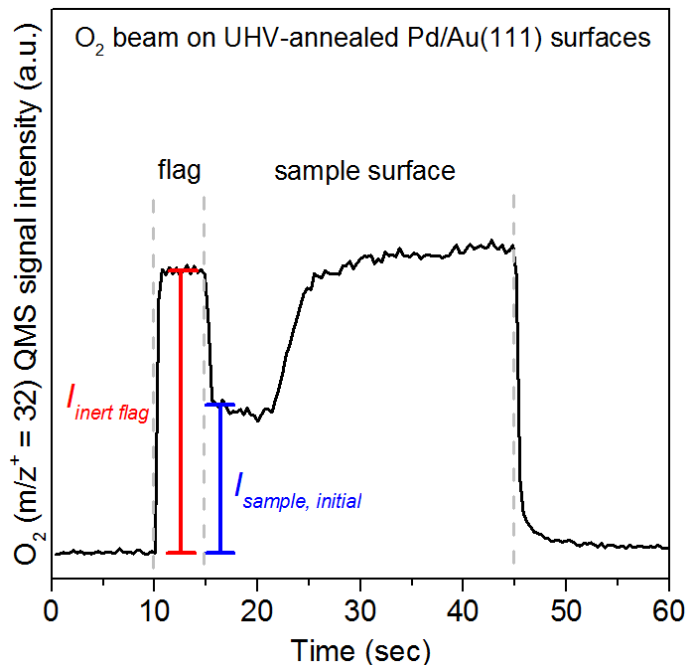


Figure S2. Calculation of initial sticking probability of O₂ on the annealed Pd/Au(111) surface using the King–Wells measurement at 77 K. The 1.5 ML Pd/Au(111) surface annealed at 500 K in UHV was used as an example surface.

The initial sticking probability of O₂ (S_{O_2}) on the surface can be calculated by (eq. S1)

$$S_{O_2} = \frac{I_{inert\ flag} - I_{sample,\ initial}}{I_{inert\ flag}} \quad (\text{eq. S1})$$

where $I_{inert\ flag}$ is the intensity of O₂ QMS signal from impingement of the O₂ beam onto the inert flag, and $I_{sample,\ initial}$ is the initial intensity of O₂ QMS signal from impingement of the O₂ beam onto the sample.

3. Calculation of O₂ uptake on Annealed Pd/Au(111) Surface during O₂ King–Wells Measurement

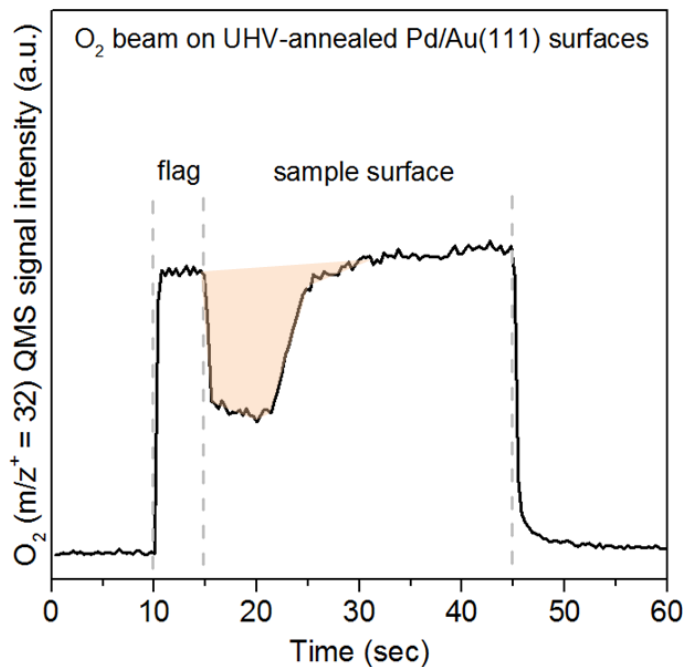


Figure S3. Calculation of O₂ uptake on oxygen-annealed 1.5 ML Pd/Au(111) surfaces during the King–Wells measurement at 77 K. The 1.5 ML Pd/Au(111) surface annealed at 500 K in UHV was used as an example surface. The O₂ uptake on the surface is proportional to the shaded area indicated in the figure.