Electronic Supplementary Information

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

Wen-Yueh Yu, Liang Zhang, Gregory M. Mullen, Edward J. Evans Jr., Graeme Henkelman and C. Buddie Mullins*

McKetta Department of Chemical Engineering and Department of Chemistry, Center for Nano and Molecular Science and Technology, Texas Materials Institute, Center for Electrochemistry, and Institute for Computational Engineering and Sciences, University of Texas at Austin, Austin, Texas 78712-0231, United States

*Corresponding author. Email: mullins@che.utexas.edu; Phone: 1-512-471-5817
1. AES Characterizations for Annealed Pd/Au(111) Surfaces

![AES spectra of 1.5 ML Pd/Au(111)](image)

**Figure S1.** AES spectra of 1.5 ML Pd/Au(111) (a) immediately after annealing in $1 \times 10^{-6}$ Torr of O$_2$ to 500 K for 10 min, and (b) after heating (a) surface to 500 K to desorb O$_2$. 
2. Calculation of Initial Sticking Probability of $O_2$ on Annealed Pd/Au(111) Surface in $O_2$ King–Wells Measurement

Figure S2. Calculation of initial sticking probability of $O_2$ 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 $O_2$ \( S_{O_2} \) on the surface can be calculated by (eq. S1)

\[
S_{O_2} = \frac{I_{\text{inert flag}} - I_{\text{sample, initial}}}{I_{\text{inert flag}}} \tag{eq. S1}
\]

where \( I_{\text{inert flag}} \) is the intensity of $O_2$ QMS signal from impingement of the $O_2$ beam onto the inert flag, and \( I_{\text{sample, initial}} \) is the initial intensity of $O_2$ QMS signal from impingement of the $O_2$ beam onto the sample.
3. Calculation of O\textsubscript{2} uptake on Annealed Pd/Au(111) Surface during O\textsubscript{2} King–Wells Measurement

**Figure S3.** Calculation of O\textsubscript{2} 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 O\textsubscript{2} uptake on the surface is proportional to the shaded area indicated in the figure.