Supplementary Information for Atomic Hydrogen Reactions of Alkanethiols on Au(111): Phase Transitions at Elevated Temperatures

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Image Line Scans

Phase Coexistance



Figure S1: STM image of a 100 nm \times 100 nm area showing ϵ regions existing with ϕ regions after 10 seconds of hydrogen exposure The blue line shows where the line scan in Figure S2

Gold Island Height

After surfaces are reacted, gold islands are left behind. The gold islands are identified by the step height of gold which is 2.35 Å.¹ An image scan be seen in Figure S3 of an 1-octanethiol surface after hydrogen exposure. The blue line on the image represents where the line graph in Figre S4. The islands are the same height as the terrace step, thus confirming the islands are gold.

Image Masks

In order to evaluate our kinetic model, the decay and growth of the ϕ and ϵ respectively. Due to the nature of the ϵ phase, it is difficult to use a program to distinguish between the



Figure S2: Line scan of Figure S1, showing the height difference between the ϕ and ϵ phases.

two phases. The surface coverage values had to be determined by manually masking the phases. This introduces bias so original images and masked images were included side by side.



Figure S3: STM image of a 125.0 nm \times 125.0 nm area showing a sample after complete hydrogen reaction. There are only gold islands remaining on the surface. The blue line shows where the line scan in Figure S4



Figure S4: Line scan of Figure S3. The change in height between the islands and the step are the same, confirming the identity of the islands



Figure S5: Surface coverage of both ϕ and ϵ over hydrogen exposure time.



Figure S6: STM image of the same 75.0 nm \times 75.0 nm area of 0 seconds of hydrogen exposure with (left) and without (right) masks. ϕ areas are marked in blue and ϵ is marked in red.



Figure S7: STM image of the same 75.0 nm \times 75.0 nm area of 10 seconds of hydrogen exposure with (left) and without (right) masks. ϕ areas are marked in blue and ϵ is marked in red.



Figure S8: STM image of the same 75.0 nm \times 75.0 nm area of 20 seconds of hydrogen exposure with (left) and without (right) masks. ϕ areas are marked in blue and ϵ is marked in red.



Figure S9: STM image of the same 75.0 nm \times 75.0 nm area of 30 seconds of hydrogen exposure with (left) and without (right) masks. ϕ areas are marked in blue and ϵ is marked in red.



Figure S10: STM image of the same 75.0 nm \times 75.0 nm area of 40 seconds of hydrogen exposure with (left) and without (right) masks. ϕ areas are marked in blue and ϵ is marked in red.



Figure S11: STM image of the same 75.0 nm \times 75.0 nm area of 50 seconds of hydrogen exposure with (left) and without (right) masks. ϕ areas are marked in blue and ϵ is marked in red.



Figure S12: STM image of the same 75.0 nm \times 75.0 nm area of 60 seconds of hydrogen exposure with (left) and without (right) masks. ϕ areas are marked in blue and ϵ is marked in red.



Figure S13: STM image of the same 75.0 nm \times 75.0 nm area of 70 seconds of hydrogen exposure with (left) and without (right) masks. ϕ areas are marked in blue and ϵ is marked in red.



Figure S14: STM image of the same 75.0 nm \times 75.0 nm area of 80 seconds of hydrogen exposure with (left) and without (right) masks. ϕ areas are marked in blue and ϵ is marked in red.





Figure S15: STM image of the same 75.0 nm \times 75.0 nm area of 90 seconds of hydrogen exposure with (left) and without (right) masks. ϕ areas are marked in blue and ϵ is marked in red.



Figure S16: STM image of the same 75.0 nm \times 75.0 nm area of 100 seconds of hydrogen exposure with (left) and without (right) masks. ϕ areas are marked in blue and ϵ is marked in red.

References

 Kautz, N. A.; Kandel, S. A. Alkanethiol/Au(111) self-assembled monolayers contain gold adatoms: Scanning tunneling microscopy before and after reaction with atomic hydrogen. *Journal of the American Chemical Society* 2008, 130, 6908–6909.