Nucleation Stage for the Oriented Growth of Tantalum Sulfide Monolayers on Au(111)

T. Chagas,[1,*] K. Mehlich,[1] A. Samad,[2] C. Grover,[1] D. Dombrowski,[1,3] J. Cai,[1] U. Schwingenschlögl[2] and C. Busse[1]

[1] *Department Physik, Universität Siegen, Walter-Flex-Str. 3, 57072, Siegen, Germany*
[2] *Physical Science and Engineering Division, King Abdullah University of Science and Technology, 23955-6900, Thuwal, Saudi Arabia*
[3] *Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149, Münster, Germany*

thais.chagas@uni-siegen.de

We study the nucleation stage in the epitaxial growth of monolayer TaS_2 as a model system for monolayer transition metal sulfides [1]. The growth was done under ultra-high vacuum conditions with Au(111) as a substrate on which the metal atoms are evaporated, and the sulfur is provided from a background of H_2S. Using scanning tunneling microscopy (STM), we find atomic-scale protrusions with a well-defined triangular shape that act as nuclei for the further growth of extended tantalum sulfide monolayers (figure 1, left panel). We identify these protrusions as TaS_3 (figure 1, right panel) using density functional theory (DFT). We propose that their unique orientation is the cause of the well-defined orientation of a complete TaS_2 layer found under favorable growth conditions [2].

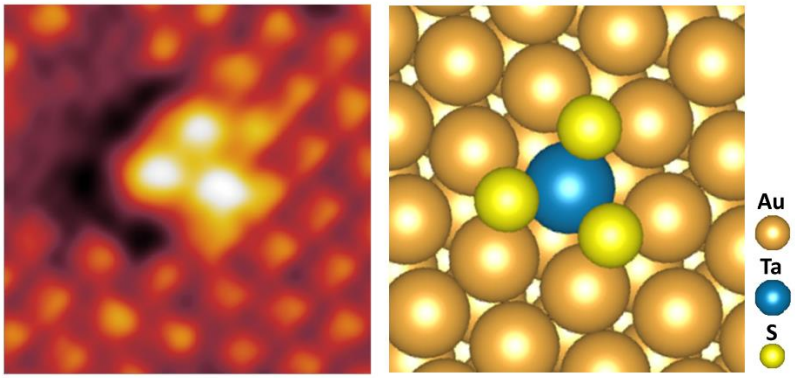

Fig. 1. (Left panel) Atomically-resolved STM topographic image of the protrusions (appearing as three dots) on Au(111). Image parameters: 1.9 nm × 1.9 nm, U = -0.3 V, I = 2.3 nA. (Right panel) Structural configuration of TaS_3 (top view) with a Ta atom (shown in blue) embedded in the Au(111) substrate (shown in gold) and connected to three S atoms (shown in yellow).

[1] Chagas, T., Mehlich, K., Samad, A., Grover, C., Dombrowski, D., Cai, J., Schwingenschlögl, U., Busse, C. *J. Phys. Chem. C,* **127**, 5622 (2023). DOI: 10.1021/acs.jpcc.3c00234
[2] Dombrowski, D. Samad, A., Mehlich, K., Chagas, T., Schwingenschlögl, U., Busse, C. *2D Mater.* **10**, 025005 (2023). DOI: 10.1088/2053-1583/acb279