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Self-Assembly of Thiol Adsorbates on the Au(111)surface FRANK HAGELBERG, QUINTON WILLIAMS, JIAN-GE ZHOU, Jackson State University — A long-standing controversy related to the dimer pattern formed by methanethiol (CH3SH) and methylthiolate (CH3S) on the Au(111) surface has been resolved using density functional theory within periodic boundary conditions. It is found that the S atoms of methanethiol adsorbates on the Au(111) surface form Van der Waals dimers. For methylthiolate, it is shown that no dimerization occurs at high coverage. At intermediate coverage, however, a Van der Waals dimer pattern emerges. The presence of defects in the Au(111) surface does not change this conclusion. Molecular dynamics simulation at high coverage demonstrates that the observed dialkyl disulfide species emerge during the desorption process, and thus are not attached to the surface. A meta-stable monomer pattern has been shown to be only marginally higher in adsorption energy than the dimer configuration which explains the observed fragility of the dimers. For the understanding of these results, it is of crucial importance that methanethiol molecules, contrary to a widely held assumption, remain stable when deposited on clean Au(111) surfaces /1, 2/. In the presence of defects, however, methanethiol adsorbates dissociate and form methylthiolate. /1/ I. Rzeznicka, J. Lee, P. Maksymovych, J. Yates, Jr., J. Phys. Chem. B109, 15992 (2005). /2/ J. Zhou, F. Hagelberg, Phys. Rev. Lett. 97, 45505 (2006).

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