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A combined theoretical and experimental study on the structure of Methylthiolates on the Au(111) surface RICCARDO MAZZARELLO, R. ROUSSEAU, SISSA and ICTP, Trieste, Italy, S. SCANDOLO, ICTP, Trieste, Italy, A. VERDINI, A. COSSARO, TASC-INFM, Trieste, Italy, L. CASALIS, Sincrotrone, Trieste, Italy, L. FLOREANO, A. MORGANTE, TASC-INFM, Trieste, Italy, M. F. DANISMAN, Princeton University, USA, G. SCOLES, SISSA, Trieste, Italy and Princeton University, USA — Self-assembled monolayers (SAMs) of sulphur containing organic molecules on gold have received enormous attention due to the central role these interfaces play in molecular electronic devices, biosensors, surface coatings and nanolithography. Despite their interest the atomic structure of Methylthiolates on Au(111) surfaces, the simplest SAM in this class, is not fully understood. Here we address this problem with a combined theoretical and experimental study. We show that an asymmetric bridge (quasi on-top) site fits both the X-Ray and Photoelectron Diffraction data better than either the symmetric bridge site or on-top site. To understand this phenomenon we have performed molecular dynamics simulations employing density functional theory within the generalized gradient approximation. We show that at high temperatures the presence of vacancies and gold adatoms tends to favour the quasi on-top site, in spite of the fact that the symmetric bridge site is the lowest energy site at $T = 0$.

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