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Density functional theory study of the energetics of SH molecules on Au (111) and the threshold coverage for surface reconstruction lifting YONGDUO LIU, VIDVUDS OZOLINS, University of California Los Angeles Department of Materials Science — The structure of self-assembled monolayers of SH molecules on Au (111) has been studied within both low and high coverage regimes. A dumbbell-like structure is favorable in energy over any other possible surface morphology in the low coverage regime. At full coverage, a structure is proposed that is similar to that of the c (4x2) structure, but at twice the size. In addition, we also investigate the adsorbent-mediated Au herringbone reconstruction lifting. Results show that the threshold coverage for the lifting is 0.47 monolayer, with the mechanism being attributed to the interactions between the intrinsic dipole moments of the surface and SH molecules.

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