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Surface Reconstruction Transition Induced by Adsorption of Molecules: Perylene and FePc on Au(111) Surface JIATAO SUN, L. GAO, S. X. DU, F. LIU, Department of Materials Science and Engineering, University of Utah, USA, H.-J. GAO, Institue of Physics, Chinese Academy of Sciences, Beijing — Gold is the most commonly used electrode material in molecular electronics. It is well known that real Au(111) surface will reconstructs into a 22 $\times\sqrt{3}$ herringbone structure at ambient conditions. The stability of the Au(111) surface reconstruction is subject to changing under many conditions. Thus fabrication of high-quality organic thin films on metal surfaces is one crucial issue in molecular electronics. New Au(111) surface reconstruction patterns have been observed by STM upon the adsorption of monolayer perylene ($C_{20}H_{12}$) and monolayer iron phthalocyanine ($C_{32}H_{16}N_8Fe$) respectively. First-principles calculations and Frenkel-Kontorova model have been used to investigate the physical mechanism. Stress anisotropy has been found to be the main factor driving the transition of surface reconstruction. The difference in strength of the interaction between molecules and the gold substrate, may lead to different stress anisotropy for both systems. These results will be very useful to transport properties in electronic devices.

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