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Effects of Embedded Dipoles on the Electrical Response of Self Assembled Monolayers P.P. ZHANG, O.M. CABARCOS, T.A. DANIEL, P.S. WEISS, D.L. ALLARA, The Pennsylvania State University — There has been recent interest in the use of polar molecules assembled at electrodes for tuning work functions and engineering charge injection barriers in organic electronic devices. With this in mind we have been investigating the electrostatic properties of simple model systems prepared from self-assembled alkanethiolate monolayers on Au{111} with the incorporation of an embedded ester moiety [-(CO₂)- = E] in the adsorbate molecules. The intrinsic static dipole moment of the ester moiety of ~1 Debye magnitude leads to the formation of a strong, highly organized, planar electric dipole layer in the SAM. From our previous X-ray photoelectron spectroscopy data we observe a consistent shift of the C 1s photoelectron kinetic energies between the top and bottom alkyl segments, defined as -(CH₂)_m-E-(CH₂)_nCH₃, regardless of the relative lengths *m* and *n*. This shift correlates well with the value of the electrostatic potential across the E layer. Our recent surface potential AFM measurements, however, reveal an apparently anomalous strong dependence of surface potential on the sizes and ratios of *m* and *n*, in contrast to the constant electrostatic potential observed in XPS measurements. Mechanisms underlying these effects will be discussed, with possible implications for the electrostatic behavior of more complicated organic and biological systems.

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