

Abstract Submitted
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Engineering of the Static Interface Dipole in Metal/Organic Nanohybrid Materials¹ AXEL ENDERS, DONNA KUNKEL, JUSTIN NITZ, PETER DOWBEN, University of Nebraska - Lincoln, LUCIE ROUTABOUL, BERNARD DOUDIN, PIERRE BRAUNSTEIN, Université de Strasbourg, Strasbourg, France, SCOTT SIMPSON, EVA ZUREK, Dept. of Chemistry, SUNY Buffalo — We studied small molecules with large intrinsic electrical dipole as model system for molecular films adsorption on surfaces for altering the interface dipole screening. More specifically, we investigated the self-assembly and electronic interface properties of zwitterionic molecules of type $C_6H_2(\dots NHR)_2(\dots O)_2$ ($R = H, \dots$), adsorbed on Cu(111), Ag(111), Au(111) surfaces with scanning tunneling microscopy in UHV. These molecules carry positive and negative charges on opposite parts of the molecule, resulting in a large electric dipole of typically 10 Debye. We find that the dipole of the surface-supported molecule is decreased with respect to free species and of order of 1 - 2 Debye, depending on the substrate material. The molecules self-assemble into 2D structures upon adsorption, where the substrate-dependent strength of the dipolar interactions between the adsorbed molecules dictates the network architecture. DFT calculations were performed to analyze adsorption geometry, charge transfer and dipole moment. We will show that zwitterionic molecules provide a unique opportunity to engineer the interface dipole in metal/organic hybrid structures, which ultimately controls the charge injection barrier in devices.

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