Abstract Submitted
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Theory of work function tuning via mixed-monolayers on functional surfaces[1] MICHELE KOTIUGA, Physics Department, UC Berkeley & The Molecular Foundry, LBNL,, PIERRE DARANCET, The Center for Nanoscale Materials, ANL, JEFFREY B. NEATON, Physics Department, UC Berkeley, The Molecular Foundry, LBNL & Kavli Energy NanoSciences Institute at Berkeley, Berkeley, CA — Self-assembled monolayers (SAMs) provide both stability and functionality of surfaces useful in optoelectronic nanoscale devices. The work function, level alignment and other electronic properties of functionalized surfaces can be tuned with the choice of molecule and an even finer control of the properties can be obtained with a SAM comprised of multiple types of molecules [1]. Modeling the effect on electronic properties of mixed-monolayers via ab initio calculations poses a challenge due to the large supercell required to capture a range of relative concentrations between the two types of molecules. Here, we present an implicit model - fit from density functional theory calculations - capturing local electrostatic interactions within the SAM primarily due to depolarization of the induced dipoles formed upon binding [2]. This quantitative model allows us to explore supercells with a large number of molecules and, thus, surface concentrations that are inhomogeneous in nature. We compare to experimental results of thiol terminated carboranes on gold [1]. [1] Kim et al., Nano Lett. 14, 2946 (2014) [2] Kotiuga et al., Nano Lett. 15, 4498 (2015)

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