

Abstract Submitted  
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**Interplay between Self-Assembled Structures and Energy Level Alignment of Benzenediamine on Au(111) Surfaces<sup>1</sup>** GUO LI, Lawrence Berkeley Natl Lab, JEFFREY NEATON, Lawrence Berkeley Natl Lab; UC-Berkeley; Kavli Energy NanoSciences Institute at Berkeley — Using van der Waals-corrected density functional theory (DFT) calculations, we study the adsorption of benzene-diamine (BDA) molecules on Au(111) surfaces. We find that at low surface coverage, the adsorbed molecules prefer to stay isolated from each other in a monomer phase, due to the inter-molecular dipole-dipole repulsions. However, when the coverage rises above a critical value of  $0.9\text{nm}^{-2}$ , the adsorbed molecules aggregate into linear structures via hydrogen bonding between amine groups, consistent with recent experiments [Haxton, Zhou, Tamblyn, et al, Phys. Rev. Lett. 111, 265701 (2013)]. Moreover, we find that these linear structures at high density considerably reduces the Au work function (relative to a monomer phase). Due to reduced surface polarization effects, we estimate that the resonance energy of the highest occupied molecular orbital of the adsorbed BDA molecule relative to the Au Fermi level is significantly lower than the monomer phase by more than 0.5 eV, consistent with the experimental measurements [DellAngela, Kladrnik, and Cossaro, et al., Nano Lett. 10, 2470 (2010)].

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