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Energy Level Alignment at the Interface between Linear-Structured Benzenediamine Molecules and Au(111) Surface GUO LI, TONATIUH RANGEL, ZHENFEI LIU, Lawrence Berkeley Natl Lab, VALENTINO COOPER, Oak Ridge Natl Lab, JEFFREY NEATON, Lawrence Berkeley Natl Lab; UC-Berkeley; Kavli Energy NanoSciences Institute at Berkeley — Using density functional theory with model self-energy corrections, we calculate the adsorption energetics and geometry, and the energy level alignment of benzenediamine (BDA) molecules adsorbed on Au(111) surfaces. Our calculations show that linear structures of BDA, stabilized via hydrogen bonds between amine groups, are energetically more favorable than monomeric phases. Moreover, our self-energy-corrected calculations of energy level alignment show that the highest occupied molecular orbital energy of the BDA linear structure is deeper relative to the Fermi level relative to the isolated monomer and agrees well with the values measured with photoemission spectroscopy. This work supported by DOE.

Guo Li
Lawrence Berkeley Natl Lab

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