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Electron Binding Energies in DNA Modified Surfaces: Theory and Experiment JAMES SULLIVAN, Virginia Commonwealth University, DMITRI PETROVYKH, University of Maryland-College Park, Naval Research Lab, GEORGE SCHATZ, Northwestern University, LLOYD WHITMAN, Naval Research Lab — X-ray photoelectron spectroscopy is emerging as a powerful method for characterizing DNA on surfaces.[1] The relative positions of core electron binding energies (CBEs) suggest likely binding geometries and strength of chemical bonds, and the peak areas provide a quantitative measure of the coverage. Although CBEs for simple molecules can often be readily assigned to specific adsorption sites and bonding configurations based on historical data, such interpretation for CBEs of DNA is not generally possible. We are using density functional theory to determine the geometric and electronic configuration of DNA nucleobases, nucleosides, and nucleotides. We find the theoretical XPS spectra for isolated nucleic components are surprisingly similar to experimental spectra measured on DNA films, suggesting that—although the films are adsorbed on the surface—the underlying electronic structure of the nucleobases is "free-like." 1. D. Y. Petrovykh, et al., J. Am. Chem. Soc. 125, 5219 (2003); D. Y. Petrovykh, et al., Langmuir 20, 429 (2004).

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