## Abstract Submitted for the MAR07 Meeting of The American Physical Society

Characterization of Electrical Devices Based Upon Organic Monolayers Directly Attached to Si. C.A. RICHTER, C.A. HACKER, N. GERGEL-HACKETT, L.J. RICHTER, T.C. ALLISON, NIST, Gaithersburg, MD, V. MUJICA, Northwestern Univ, Dept Chem, Evanston, IL, C.A. GONZALEZ, NIST, Gaithersburg, MD — We present the results of electrical measurements of alkane monolayers directly attached to Si-substrates. Molecular electronic test structures consisting of thiol or alcohol terminated molecules covalently attached via UV-assembly to Si (n-type, p-type, <100>, or <111>) in oxide defined "wells" were characterized by capacitance-voltage and current-voltage (IV) measurements. These results are compared to models based on a first-order expansion of the system's Green function and a new method for the Si-molecule contact that predict a negative differential peak in the IV measurements due to an alignment between the Fermi energy of the Si substrate and the molecular LUMO. The structure of the molecular monolayers under full metallization was assessed with a novel backside incident FTIR technique and depth-profiling XPS. Au fully displaces the molecular monolayers (and forms a silicide), while Ag does not react with the underlying Si and forms a Ag/molecule/Si junction.

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