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Electrical properties of metal-molecule-silicon structures with varying molecular backbones, dipoles, and atomic tethers CURT A. RICHTER, NADINE GERGEL-HACKETT, MARIONA COLL, CHRISTINA A. HACKER, Semiconductor Electronics Division, NIST — We present the results of an extensive experimental investigation of metal-monolayer-silicon junctions. By varying the molecular dipole, the molecular backbone, the Si-molecule linkage, and the Si-doping, we indentified critical features that determine the electrical transport and injection properties of the junctions. Two basic structures were used. One is an enclosed planar structure in which an organic monolayer is directly assembled on silicon and contacted with evaporated silver. The other was made via Flip Chip Lamination, a novel approach that relies on the formation of monolayers on a gold surface first, which enables the study of a wider range of molecular layers on silicon of very high-quality. Two charge transport regimes dominate: (1) a Schottky barrier limited regime where the molecular dipole results in silicon band bending at the junction interface, and (2) a tunneling regime where the molecular dipole creates a small local electric field that screens the electrical transport. Transition Voltage spectroscopy was used to identify electrical differences between π-conjugated and alkyl backbones attributed to the extended π-delocalization and variations due to the chemical nature of Si-atom linkage.

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