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Self-Assembling Pi-conjugated Monolayer on Silicon J.-C. LIN, J. KELLAR, J.-H. KIM, S. NGUYEN, M. HERSAM, M. BEDZYK, Northwestern University, K. BEVAN, Purdue University — Pi-conjugated molecules play an important role in molecular electronic applications. For conductivity, the intrinsic ordering of the structure strongly influences its efficiency but is difficult to characterize by conventional scanning probe and IR spectroscopy techniques. In the present study, we combine a compliment of techniques, including XSW(X-ray standing waves), AFM, XPS, XRR(X-ray reflectivity), XRF(X-ray fluorescence), and DFT(Density functional theory) to determine the atomic scale molecular configurations and packing densities of two self-assembled aromatic monolayers (SAMs) grown on H-passivated silicon. P-4-bromophenyl-ethynyl-phenyl-acetylene, which has two phenyl rings, is directly compared with p-4-bromophenyl-acetylene, which has only one phenyl ring. The results show a local dense packing in spite of the overall coverage being somewhat less than 0.5 monolayers. This packing of the p-4-bromophenyl-ethynyl-phenyl-acetylene SAM suggests the average spacing between molecules is within the pi-pi interaction range, which will contribute to the charge transport. The detailed atomic structure of SAMs are also constructed using our characterization package. The result suggests the possibility of the application of self-assembling method on the growth of molecular electronics.

J.-C. Lin
Northwestern University

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