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X-ray Atomic-Scale Analysis of Self-Assembled Monolayer Growth on Silicon J.C. LIN, J. KELLAR, J. KIM, N. YODER, K. BEVAN, S. DATTA, S. NGUYEN, M. HERSAM, M. BEDZYK — Organic functionalization of silicon is of interest for applications ranging from biosensing to molecular electronics. The efficiency of molecular devices heavily depends on the ordering of the structure. Traditionally spectroscopy is used to characterize bonding, but often the overall structure can be ambiguous. Our strategy is to combine a compliment of techniques, including AFM, XPS, XRR(X-ray reflectivity), XSW(X-ray standing wave), XRF(X-ray fluorescence), and DFT(Density functional theory) to determine the atomic scale molecular configuration and packing density of Self-Assembled Monolayers (SAMs) grown on H-passivated Silicon. Our periodic DFT study of 4-bromo-phenyl-acetylene (BPA) predicts that the local packing density can affect the Br height by as much as 2 angstrom. XSW, which is used to measure the 3D Br distribution shows that the local structure is unchanged when the average SAM coverage is increased. This indicates the type of 2D island nucleation growth process being observed. Comparison between 4-bromostyrene (BrSty) and BPA SAMs provides direct evidence that the double bond root of the BPA contributes to a stiffer configuration than the single bond root. With the aromatic rings in the structure for conducting electrons, BrSty and BPA molecules are a starting point for future molecular electronic designs with more complex molecules.

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