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Orientation of Pentacene Molecules on SiO_2: From a Monolayer to the Bulk FAN ZHENG, Department of Physics, University of Wisconsin Madison, BYOUNG-NAM PARK, SOONJOO SEO, PAUL G. EVANS, Materials Science Program and Department of Materials Science and Engineering, University of Wisconsin Madison, FRANZ J. HIMPSEL, Department of Physics, University of Wisconsin Madison — The orientation of pentacene films on SiO_2 is studied for the thickness range from a monolayer to 150 nm by polarization-dependent NEXAFS spectroscopy (Near Edge X-ray Absorption Fine Structure). All films exhibit a strong polarization dependence of the π^* orbitals, which indicates that the pentacene molecules are highly oriented. However, the degree of orientation varies with the rate at which pentacene molecules are deposited. This difference can be explained by a previously-proposed mixture of the bulk phase and a metastable thin film phase. Faster rates favor the thin film phase and slower rates the bulk phase. Our NEXAFS results extend previous structural observations down to the first layer at the oxide interface, which is critical for the performance of devices. Including a finite distribution of the molecular tilt angles in the data analysis accounts for residual disorder. Damage to the molecules by hot electrons from soft x-ray irradiation eliminates the splitting between nonequivalent π^* orbitals, indicating a breakup of the pentacene molecule.

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