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Scanning Tunneling Microscopy and Spectroscopy of Thin Films of the Organic Semiconductor Picene SIMON KELLY, GEOFFREY ROJAS, PETRO MAKSYMOVYCH, Oak Ridge National Laboratory, CNMS COLLABORATION — Characterizing organic semiconductors at the single molecule scale has greatly enhanced our understanding of intermolecular interactions, revealing new approaches to controlling film structure, while probing the electronic properties of organic interfaces. Pentacene has long been a model system for such studies. Here we study monolayer and bilayer films of picene, a structural isomer of pentacene. We grow these films on Ag(111) by thermal evaporation in UHV and measure them in-situ using a low-temperature STM at $\sim$ 77 K. Topographic STM measurements were used to establish the film structure. Much like pentacene, picene bonds with its molecular plane parallel to the surface, but unlike pentacene, picene forms dimers. Moreover, the work-function shift amounts to almost 1 eV (up to 2x the value for pentacene), suggesting that the molecule-surface distance is closer in this case. At the same time, the splitting of the LUMO, LUMO+1, and LUMO+2 molecular orbitals is somewhat larger than even semiempirically calculated values for the gas-phase. These measurements will be compared to first principles calculations made with the HSE functional to understand changes to the electronic structure with adsorption and the role of van-der-Waals interactions between flat-lying picene molecules.

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