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Scanning Tunneling Microscopy and Spectroscopy of Thin Films
of the Organic Semiconductor Picene SIMON KELLY, GEOFFREY ROJAS,
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RATION — 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 ~ 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 molecu-
lar 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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