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Anchoring and Bending of Pentacene on Aluminum (001) GUIDO FRATESI, ETSF, CNISM, Dip. di Fisica, Università di Milano, Via Celoria 16, I-20133 Milano, Italy, and Dip. di Scienza dei Materiali, Milano-Bicocca, ANU BABY, Dipartimento di Scienza dei Materiali, Università di Milano-Bicocca, Via Cozzi 55, I-20125 Milano, Italy, SHITAL R. VAIDYA, LAERTE L. PATERA, CNR-IOM, Lab TASC, Dep. of Physics, and Grad. School of Nanotechnology, Univ. of Trieste, Via Valerio 2, I-34127 Trieste, Italy, CRISTINA AFRICH, LUCA FLOREANO, CNR-IOM, Laboratorio TASC, Basovizza SS-14, Km 163.5, I-34149 Trieste, Italy, GIAN PAOLO BRIVIO, ETSF, CNISM, Dipartimento di Scienza dei Materiali, Università di Milano-Bicocca, Via Cozzi 55, I-20125 Milano, Italy — We study the structural, electronic, and spectroscopic properties of pentacene adsorbed on Al(001) surface, combining density functional theory (DFT) methods including van der Waals interactions with x-ray photoemission (XPS), near-edge x-ray absorption fine structure (NEXAFS), and scanning tunneling microscopy (STM). We find a major change of the molecular backbone resulting into a peculiar V-shape bending, due to the direct anchoring of the two central carbons atop two Al atoms underneath. In the most stable adsorption configuration, pentacene is oriented with the long axis parallel to the substrate [110] direction, where such anchoring is favored by optimally matched interatomic distances. Remarkably, due to the generally low degree of order, we measure by STM a significant portion of molecules oriented along the [100] direction, which also display the same V-shape conformation, as driven by the link of the central carbon atoms of pentacene to a pair of slightly displaced Al atoms.

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