

Intermolecular band dispersion in quasi-one-dimensional adenine assemblies

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Electronic Supplementary Information

Experimental

Adenine (Sigma, purity > 99%) has been thoroughly degassed *prior* to the deposition onto HOPG (0001) substrates (ZYA quality, NT-MDT) that were cleaved in air and heated at 400 °C for 12 h. Molecules have been deposited in UHV at a rate of about 0.05 Å/min, the substrates held at 40 °C. The films were exposed to a partial water vapor pressure of about 10^{-4} mbar for 15 min, as described previously [14].

The base pressure of the UHV systems used is better than 3×10^{-10} mbar. Following each preparation step, films held at 298 K were characterized by UPS in a home-based set-up, using He I radiation (21.2 eV). In the home-based set-up, the energy resolution is better than 30 meV. The work function was derived from the secondary electron cut-off of the He I spectra, the sample biased at -5.0 V.

Photon-energy dependent UPS measurements were performed in normal emission geometry at the ISSP beamline BL-18A of the Photon Factory synchrotron radiation facility (KEK, Tsukuba, Japan) equipped with a SCIENTA SES-100 analyzer. The position of the Fermi level was determined from a nearby mounted metal plate. For photon energies between 35 and 65 eV, the total energy resolution varies between about 130 and 230 meV. Spectra were obtained at normal emission using linearly-polarized light, the angle integrated within $\pm 2^\circ$.