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Orbital tomography: Deconvoluting photoemission spectra of organic molecules[1] PETER PUSCHNIG, University of Leoben, EVA-MARIA REINISCH, THOMAS ULES, GEORG KOLLER, University of Graz, Austria, SERGEY SOUBATCH, Forschungszentrum Juelich, Germany, MARKUS OSTLER, University Erlangen-Nuernberg, Germany, LORENZ ROMANER, University of Leoben, Austria, F. STEFAN TAUTZ, Forschungszentrum Juelich, Germany, CLAUDIA AMBROSCH-DRAXL, Humboldt University Berlin, Germany, MICHAEL G. RAMSEY, University of Graz, Austria — We study the interface of an organic monolayer with a metallic surface, *i. e.*, PTCDA (3,4,9,10-perylene-tetracarboxylic-dianhydride) on Ag(110), by means of angle-resolved photoemission spectroscopy (ARPES) and *ab initio* electronic structure calculations. We present a tomographic method which uses the energy and momentum dependence of ARPES data to deconvolute spectra into individual orbital contributions beyond the limits of energy resolution. This provides an orbital-by-orbital characterization of large adsorbate systems without the need to invoke sophisticated theory of photoemission, allowing us to directly estimate the effects of bonding on individual orbitals. Moreover, this experimental data serves as a most stringent test necessary for the further development of *ab initio* electronic structure theory.

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