

Abstract Submitted
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Inter- and intramolecular dispersion in a highly ordered organic molecular crystal.¹ STEPHEN BERKEBILE, KF University, 8010 Graz, Austria, PETER PUSCHNIG, Montan University, Leoben, Austria, GEORG KOLLER, FALKO P. NETZER, MICHAEL G. RAMSEY, KF University, 8010 Graz, Austria — The inter- and intramolecular dispersion in organic molecular crystals have been predicted by theory, but never measured to a satisfying degree. Further, organic pi-conjugated molecules, as they are intrinsically one-dimensional objects with a well-defined number of repeating units, serve as a simple model for understanding what happens to the basic electronic structure in systems of limited size and low dimensions. Here, the band structure of a highly ordered and crystalline paraxiphenyl (6P) film has been measured using angle-resolved photoemission spectroscopy (ARUPS) in the three directions important to charge transport in organic devices. The ARUPS behavior reveals both strong intermolecular dispersion perpendicular to the molecular axis and intramolecular dispersion along the axis of the molecules. The data will be shown to be in very good agreement with calculations in terms of the extent of the band dispersion, the ARUPS intensity and the k-spread of the peaks associated with quantum size effects.

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