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Organic thin films with charge carrier mobility exceeding that of single crystals ZACHARY LAMPORT, OANA JURCHESCU, CYNTHIA DAY, Wake Forest University, WILLIAM MITCHELL, DAVID SPARROWE, Merck Chemicals Ltd., RUIPENG LI, DETLEF SMILGIES, Cornell University, VEACESLAV COROPCEANU, Georgia Institute of Technology — The highest reported mobilities in organic semiconductors are generally derived from single-crystal measurements where the transport is not limited by grain boundaries or mixed crystal orientations found in thin films. Because of this, single crystals are used as the benchmarks for performance of a material. Here we present an example where single crystal performance is inferior to that of thin-films. We evaluate the electrical performance of 7,14-bis-trimethylsilanylethynyl-dibenzo[a,h]anthracene from field-effect transistor measurements and find single crystal mobilities (10^{-2} cm²/Vs) two orders of magnitude lower than that obtained from thin films (1 cm²/Vs). X-ray diffraction measurements confirm that our single crystals are of high quality and exhibit a pure [001] preferential orientation of the molecules, with π - π stacking parallel to the substrate, whereas thin films display mixed [001] and [02-1] orientations. Density functional theory calculations show that the (100) direction is the main direction for hole transport. Thus, in thin-film devices we partially accessed the direction of fast transport, while in single crystals the reduced mobility is a result of the misalignment of the (100) direct lattice vector and the long axis of crystals, along which measurements were taken. Anisotropy measurements have confirmed that the high-mobility direction is not along the long axis but a different direction in the a-b plane.

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