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Understanding polymorph accessibility in molecular semiconductor thin films GEOFFREY PURDUM, Dept. of Chemical and Biological Engineering, Princeton University, THOMAS GESSNER, CHAO WU, BASF SE, GMV/T J542S, 67056, Germany, R. THOMAS WEITZ, Physics Department, Ludwig-Maximilians-Universitt Mnchen, YUEH-LIN LOO, Dept. of Chemical and Biological Engineering, Princeton University — We investigated the polymorphic stability and reversibility of thin films of a series of core-halogenated naphthalene tetracarboxylic diimides (NTCDIs) with varying alkyl substitutions. Each derivative adopts its β -phase upon thermal evaporation; post-deposition processing via solvent-vapor annealing converts the β -phase to the α -phase in two of the four derivatives. NTCDIs adopt layered structures driven by strong intralayer π - π interactions and weaker interlayer van der Waals interactions. The presence of interlayer short contacts effectively locks the structure in place, preventing any molecular reorganization upon post-deposition processing. The absence of such short interlayer contacts is instead correlated with reversible access of both polymorphs; judicious selection of post-deposition processing conditions tunes which polymorph is accessed. This finding is generalizable across a wide range of molecular semiconductors that adopt layered structures, including derivatives of benzothiophene and functionalized acenes. Beyond organic electronics, this finding has implications on pharmaceuticals and the food industry as polymorphic stability governs bioavailability and solubility.

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