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Polymorphism in Core-Chlorinated Naphthalene Tetracarboxylic Diimide Thin Films GEOFFREY PURDUM, Dept. of Chemical and Biological Engineering, Princeton University, Princeton, NJ 08544, FALK MAY, BASF SE, GVM/M - B009, 67056 Ludwigshafen, Germany, NAN YAO, Princeton Institute for Science and Technology of Materials, Princeton University, Princeton, NJ 08544, THOMAS WEITZ, BASF SE, GVE/F - J542s, 67056 Ludwigshafen, Germany, YUEH-LIN LOO, Dept. of Chemical and Biological Engineering, Princeton University, Princeton, NJ 08544 — Polymorphism within organic semiconductors can play a critical role in device performance, as some packing motifs may be more favorable to charge transport than others. As-evaporated polycrystalline thin-films of core-chlorinated naphthalene tetracarboxylic diimides (NTCDI-1) adopt a triclinic polymorph that is not different from those of single crystals grown via physical-vapor transport. Exposing these thin-films to saturated vapors of select organic solvents, such as those of acetone and chloroform, induces structural transformation; thermally evaporated films convert from the triclinic polymorph to a monoclinic polymorph that was reported for solution-grown single crystals. Isothermal transformations are well described by second-order Avrami kinetics; molecular dynamic simulations give us insight into how solvents induce different kinds of favorable molecule-molecule interactions. Interestingly, the surface energy of the underlying substrate also plays a role in determining the rate of transformation; the rate of transformation is 2x and 4x faster on hexamethyldisilazane modified-Si/SiO_2 compared to on Si/SiO_2 and octadecyltrichlorosilane modified-Si/SiO_2, respectively.

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