

Abstract Submitted
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Traversing the crystalline phase space of contorted hexabenzocoronene to maximize charge transport ANNA HISZPANSKI, Chemical and Biological Engineering, Princeton University, ARTHUR WOLL, Cornell High Energy Synchrotron Source, Cornell University, NAN YAO, PRISM Imaging and Analysis Center, Princeton University, YUEH-LIN LOO, Chemical and Biological Engineering, Princeton University — Alternative crystal structures of molecular semiconductors may exhibit increased intermolecular charge transport, but methods to controllably access non-thermodynamically-favored crystal structures are lacking. Starting with an amorphous film of contorted hexabenzocoronene (HBC) and applying thermal and solvent-vapor annealing to induce crystallization, we have accessed three distinct HBC polymorphs, two of which have previously not been observed. HBC films crystallize as polymorph I upon thermal annealing and as polymorph II upon solvent-vapor annealing with tetrahydrofuran. Subsequent solvent-vapor annealing of polymorph I converts it to polymorph II; thermal annealing of polymorph II transforms HBC to yet a different crystal structure, denoted polymorph II'. Though the crystal structure can be tuned through sequential processing, the preferred out-of-plane molecular orientation adopted by HBC is determined primarily by the first processing step. By imposing different processing sequences, we can access films having different polymorphs but the same molecular orientation, and also films having the same polymorph but different molecular orientations, thereby allowing us to decouple the relative contributions of polymorphism and preferential orientation to charge transport.

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