Tuning contorted hexabenzocoronene crystal structure and texture for organic field-effect transistors

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Crystallography conducted on single crystals reveals contorted hexabenzocoronene (HBC) can adopt either herringbone (Pbcn) or slip-stack (P21/c) packing motifs. By adjusting the molecule-solvent interactions during solvent-vapor annealing (SVA), we can controlably crystallize thin films of HBC and access both packing motifs. In HBC films annealed with dichloromethane (DCM) vapor, molecule-solvent interactions are strong and yield highly oriented Pbcn crystals. However, in films annealed with hexanes vapor, molecule-solvent interactions are weaker and randomly oriented P21/c crystals form. In addition to tuning the molecule-solvent interactions via solvent choice, the interactions may also be modulated by selectively fluorinating the peripheral aromatic rings of HBC. With increased fluorination, we decrease molecule-solvent interactions during SVA. As such, we can coax these HBC derivatives to adopt the P21/c crystal structure even with DCM SVA. Further, more fluorinated HBCs form more oriented crystals when exposed to DCM vapors. Transistors fabricated with crystalline HBC active layers suggest that the mobilities of these devices are, to first order, determined by the extent of crystal orientation and less so by the crystal structure. The ability to independently access both crystal structures with varying degrees of orientation has allowed us to decouple their relative contributions to device performance.

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