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The 2D Selfassembly of Benzimidazole and its Co-crystallization.

PAULO COSTA, JACOB TEETER, DONNA KUNKEL, ALEXANDER SINITSKII, AXEL ENDERS, University of Nebraska-Lincoln — Benzimidazoles (BI) are organic molecules that form ferroelectric crystals. Key to their ferroelectric behavior are the switchable N···HN type bonds and how they couple to the electron system of the molecules. We attempted to crystallize BI on various metal surfaces and studied them using STM. We observed that on Au and Ag, BI joins into zipper chains characteristic of its bulk structure that can pack into a continuous 2D layer. Because the dipole of BI lies in the direction of its switchable hydrogen bond, these zippers should in principle have reversible polarizations that point along the direction they run. BI's crystallization is reminiscent to how croconic acid (CA) crystallizes in 2D using O···HO bonding, suggesting that these molecules may be able to co-crystallize through OH···N bonds. This would present the opportunity to modify BI's properties, such as the energy needed to switch a hydrogen from a donor to acceptor site. When co-deposited, CA and BI successfully combine into a co-crystal formed by building blocks consisting of 2 CA and 2 BI molecules. These findings demonstrate the usefulness of using STM as a preliminary check to verify if two molecules are compatible with each other without having to attempt crystallization with multiple solvents and mixing methods.

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