Organic crystal orientation regulated by self-assembled monolayers

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We present our updated efforts to control heterogeneous nucleation of organic crystals. Selfassembled monolayers with -OH, -COOH, and $-CH_3$ functional groups were chosen as nucleating surfaces for theobromine, the primary alkaloid in chocolate. The theobromine crystals formed on the monolayer surfaces possessed distinctive orientations with respect to the nucleating surfaces. The orientational differences that originated from the variation of the crystal-surface interactions were confirmed using X-ray diffraction in the 2theta-theta mode, although these were qualitatively easy to identify in microscopic observation. The molecular interactions that regulate the orientation of theobromine are comparable to those for caffeine orientation, which we previously reported.