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A Model Study of Adlayer Pattern Formation on Square and Hexagonal Substrates HOWARD MAYNE, GENNADIY BEREZUTSKIY, GREG BUBNIS, LUCAS LAWRENCE-HURT, University of New Hampshire — In recent years there has been considerable interest in the "bottom-up" approach to nanotechnology. In particular, the self assembly of patterned templates on solid surfaces from solution or gas phase has been vigorously explored. We present here a model study to investigate pattern formation of a monolayer of linear molecules whose centers are fixed on a square (100) and hexagonal (111) substrates. The molecules interact through a realistic tip-to-tip interatomic potential energy function, whose parameters can be systematically varied. Simulations were carried out to identify the thermodynamically most stable adlayer geometry, as well as the kinetically-controlled geometry obtained via annealing. In general, we found that short-range attraction favors interactions between nearest-neighbor tips, resulting in "short stripes". Long-range attraction leads to "long stripe" geometries, where each tip interacts equally with two nearest neighbors. Intermediate-range attraction leads to a variety of structures, including several "herringbone" patterns, which depend sensitively on the interplay of attractive and repulsive forces. More detailed results will be presented, together with a discussion of candidate systems for further study.

Howard Mayne
University of New Hampshire

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