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Molecular Organization of Vapor Deposited Rod-Like Molecules
ANDREW AUDLEY, JUTTA LUETTMER-STRATHMANN, Department of Physics, The University of Akron — Thiophenes are π-conjugated organic molecules with applications in electronic devices. Alpha-sexithiophene (α-6T) is a rod-like molecule consisting of six thiophene rings. Previous experimental research has shown that vapor deposition of rod-like organic molecules onto substrates of varying temperatures yields varying material phases. These include smectic liquid crystalline phases, which have been shown to promote anisotropic charge carrier mobility. In this work, we use a course-grained model for α-6T, representing it as a chain of discotic particles with fixed bond lengths and fixed bond angles. We perform Monte Carlo simulations of multiple chains introduced at varying rates in vacuum near two adsorbing surfaces. These simulations are not chemically realistic, instead focusing on the general features of the physical systems. The goal of this work is to simulate vapor deposition of materials on a substrate under varying temperatures and deposition rates and investigate the resulting phases.

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