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Monte-Carlo simulations of a coarse-grained model for α-oligothiophenes AMANI ALMUTAIRI, JUTTA LUETTMER-STRATHMANN, Department of Physics, University of Akron — The interfacial layer of an organic semiconductor in contact with a metal electrode has important effects on the performance of thin-film devices. However, the structure of this layer is not easy to model. Oligothiophenes are small, π-conjugated molecules with applications in organic electronics that also serve as small-molecule models for polythiophenes. α-hexithiophene (6T) is a six-ring molecule, whose adsorption on noble metal surfaces has been studied extensively (see, e.g., Ref. [1]). In this work, we develop a coarse-grained model for α-oligothiophenes. We describe the molecules as linear chains of bonded, discotic particles with Gay-Berne potential interactions between non-bonded ellipsoids. We perform Monte Carlo simulations to study the structure of isolated and adsorbed molecules. [1] M. Kiel et al. Phys. Rev. B 75, 195439 (2007).

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