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Structural properties of thiophenes investigated with simulations of a coarse-grained model JUTTA LUETTMER-STRATHMANN, AMANI ALMUTAIRI, University of Akron — Thiophenes have important applications in organic electronics, energy conversion, and storage. 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. In recent work, we developed a coarse-grained model for alpha-oligothiophenes in the bulk and near gold surfaces. We describe the molecules as linear chains of bonded, discotic particles with Gay-Berne potential interactions between non-bonded ellipsoids. In this work, we investigate structural properties of thiophenes with simulations of our coarse-grained model.

Jutta Luettmer-Strathmann
University of Akron

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