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**Monte Carlo Studies of Soft Pentagonal Rotors and Polymer Self-Assembly** MICHAEL WINOKUR, University of Wisconsin, MARCUS MUELLER, Georg August Universitaet — Side chain substitution is widely used in  $\pi$ -conjugated polymers to promote processibility and reduce interchain aggregation. However this functionalization also creates diverse materials that self-organize at molecular length scales. Small modifications in the chemical architecture often produce large variations in the observed structures and phase behavior. An example of this is poly(9,9-bis(2-ethylhexyl)fluorene) (PF2/6) in which single chains form helices that subsequently undergo a supramolecular self-assembly to give a three chain unit cell or, equivalently, a  $\sqrt{3} \times \sqrt{3}$  superlattice. Direct structure studies indicate that PF2/6 incorporates a heterogeneous sequence of conformational isomers approximating a 5-fold helix and this construction defines the overall shape of the chain. In terms of more conventional polymers we consider PF2/6 to be representative of a sparse brush with, on average, a columnar type structure. However PF2/6 structure studies already indicate that the potential is not uniformly cylindrical because of the 5-fold helix and the spontaneous formation of a 3 chain unit cell. Through construction of a representative ansatz Hamilton we have mimicked the interaction between soft pentagonal shaped rotors. Monte Carlo calculations employing this Hamiltonian identify a range of parameters that reproduce the experimentally observed  $\sqrt{3} \times \sqrt{3}$  superlattice. Moreover we find that small changes in this orientational pair potential strongly alter the phase behavior.

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