Abstract Submitted
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Promotion of the Polyfluorene Beta-Phase: A First Principles Study[1] ELIZABETH M. LUPTON, FENG LIU, Department of Materials Science and Engineering, University of Utah, Salt Lake City UT-84122, DAVID G. PRENDERGAST, JEFFREY B. NEATON, The Molecular Foundry, Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley CA-94720 — Two configurations of polyfluorenes - potentially important for their blue emission properties in organic devices - have been identified in single molecule spectroscopy experiments: a glassy phase with random torsional angles between fluorene units, and a planar beta-phase. The twisted conformtaion is known to be the lowest energy structure, and the factors which promote the stabilization of the beta-phase are unclear. We present a density functional theory study of ways in which polyfluorene molecules could be manipulated to favor the formation of the photophysically more stable beta-phase. Extension along the molecular axis, which increases the stability of the planar conformation relative to the glassy phase, and the role of side groups are examined in fluorene oligomers and a polyfluorene infinite in the molecular axis. Implications for excited state properties, including fluorescence, will be discussed in the context of these results.

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