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Effect of Conformation in Charge Transport for Semiflexible Polymers RODRIGO NORIEGA, University of California Berkeley, ALBERTO SALLEO, ANDREW SPAKOWITZ, Stanford University — Current models for the electronic properties of semiconducting conjugated polymers do not include the hierarchical connectivity between charge transport units that results from the physical makeup of the materials. Concepts like on-chain vs. interchain mobility anisotropy have been known for a long time, yet they must be artificially incorporated into simulations. Models that achieve remarkable predictive power but provide limited physical insight when applied to this new class of materials are of limited use for the rational design of new conjugated polymers. Here we present a new model in which the morphology of individual polymer chains is determined by well-known statistical models and the electronic coupling between units is described using Marcus theory. Combining knowledge from polymer physics and semiconducting materials into an analytical and computational model that realistically incorporates the structural and electronic properties of conjugated polymers, it is possible to explain observations that previously relied on phenomenological models. The multi-scale behavior of charges in these materials (high mobility at short scales, low mobility at long scales) can be naturally described with our framework.

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