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Influence of Environment on the Electronic Structure of Polyfuorenes[1] ELIZABETH M. LUPTON, FENG LIU, Department of Materials Science and Engineering, University of Utah, Salt Lake City, UT 84112 USA — The influence of the structure of polyfluorene molecules on their emissive characteristics, as utilized in polymer LEDs, can be characterized using first principles methods. Here we concentrate on how factors such as external restrictions, structural and chemical defects, and constraints caused by side groups can affect the electronic structure of polyfluorenes, in particular the extent of conjugation along the backbone. Using Car – Parrinello Molecular Dynamics simulations, where the electronic structure is calculated according to Density Functional Theory 'on the fly' for a molecular dynamics trajectory, we systematically investigate how curving the backbone combined with torsional rotation between repeat units, as well as ketone defects, can affect the electronic structure. This demonstrates the way in which restrictions imposed by the environment could ultimately affect the light emitting properties of the polymer.

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Elizabeth Lupton

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