

Abstract Submitted
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Mechanical control of morphology in fluorene oligomers: First principles calculations¹ ELIZABETH M. LUPTON, FENG LIU, Department of Materials Science and Engineering, University of Utah, Salt Lake City, UT-84112 — Mechanically induced strain can have a significant impact on the optical properties of conjugated polymers. We use *ab-initio* computational methods to investigate tensile stretching and compression of polyfluorene oligomers. We show that strain can result in changes in backbone morphology which relate to shifts in transition energies in a non-trivial manner. In particular, compression of oligomers results in two distinct morphologies which shift the signal in opposite directions, despite an equal distance between terminal atoms. We also consider the application of strain through adsorption on a silicon substrate. Extension or compression can be induced through mismatch between the lattice of the substrate and the size of the repeat unit of the molecule.

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