On the Crystalline Polyfluorene Structure and Optical Spectra

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Abstract. We study the polyfluorene crystal using computational modelling based on the density functional theory. We assume a geometry with two monomers per unit cell and periodicity along the polymer's backbone structure. The stable structure determined at these conditions is characterized by significant torsion angles between individual units. We calculate its optical spectra using the TDDFT method and find a gap of 2.73 eV which is in a very good agreement with the experimental value of 2.83 eV reported in our recent paper for a thermally annealed PFO film.