Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information for: Getting excited: Challenges in quantum-classical studies of excitons in polymeric systems

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The optimized structures of DPE, Me-DPE and n-PPE (n=1,2,...,10) in MD and DFT and input files for VOTCA package for calculating excitation energies can be downloaded from our website (http://www.softsimu.net/).

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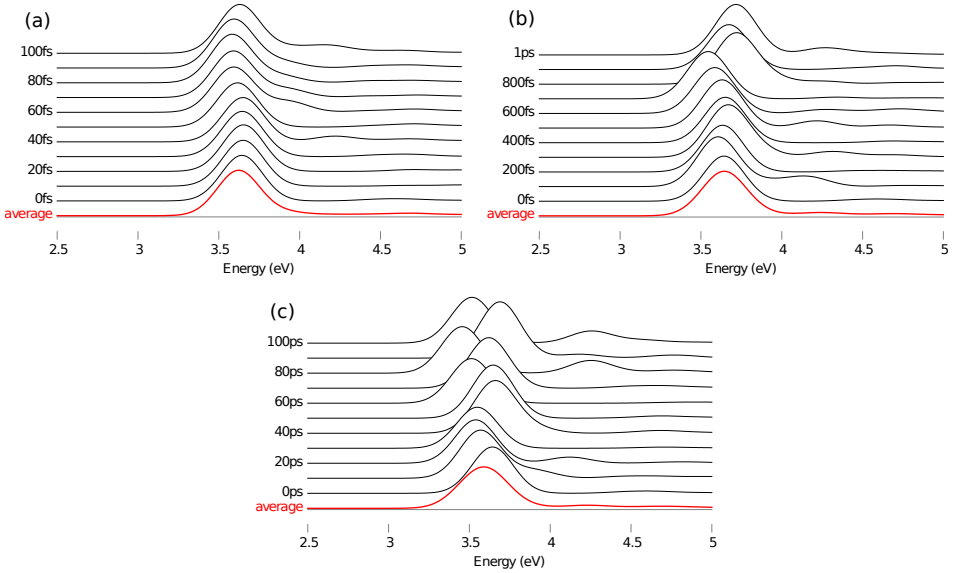

Figure 1: Optical absorption spectra for 10-PPE in toluene for time step 10 fs, 100 fs and 10 ps starting from the same starting configuration. The red curve is the average over eleven snapshots respectievely.