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 respectively.