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Molecular dynamics simulations for the study of optical properties in conjugated semiconducting molecules JACK WILDMAN, JEAN-CHRISTOPHE DENIS, PETER REPIŠČÁK, MARTIN J. PATERSON, IAN GALBRAITH, Heriot-Watt University — Conformational disorder of conjugated polymers strongly influences their optical and electronic properties. Molecular Dynamics (MD) simulations can provide a quantitative understanding of these effects. Given the ever-expanding range of molecules with potential for device applications, it is critical to systematically establish accurate MD parameters for such simulations. We present an experimentally verified, general and optimised procedure, based on a computationally inexpensive methodology for generating the required MD parameters for conjugated molecules. By combining a large sample ($\sim$1000) of MD generated conformations with DFT calculations for the resulting electronic states we can explore the influence of conformational disorder on the optical properties. Using this scheme, we determine the effect of conformational variation on both linear and two-photon absorption spectra in a number of different conjugated semiconducting oligomers. Our results indicate that, while there exists significant inhomogeneous broadening in the linear absorption, there is only a weak conformational influence on the two-photon absorption spectrum.

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