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Conformation excited-state of *o*-phenylenes by DFT method

AZUSA MURAOKA, Meiji University, JST CREST, KOICHI YAMASHITA, The University of Tokyo, JST CREST — Conjugated polymers such as polyaromatic molecules with the π/π stacking interaction have recently attracted much interest in the production and the development of the solar cell materials. Polyphenylene nanostructures are now well established in the fundamental class of conjugated polymers. This class can be divided into *para*, *meta* and *ortho* phenylenes. In previously, we have found that the ground-state structures of tetrameric *ortho* phenylenes (4-OP) have helical tightly packed *n*-phenylenes with π/π stacking interactions. In this study, in order to investigate electronic energy transfer in *ortho* phenylenes, we determine the excited-state structures and UV-visible absorption spectra in 4-OP using the density functional theory method.

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