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Accuracy of different DFT formalisms for prediction of two-photon absorption properties of conjugated polymers IFFAT NAYYAR, NanoScience Technology Center, Department of Physics, University of Central Florida, Orlando, FL-32826, IVAN MIKHAILOV, NanoScience Technology Center, University of Central Florida, Orlando, FL-32826, ARTEM MASUNOV, NanoScience Technology Center, Department of Physics, Department of Chemistry, University of Central Florida, Orlando, FL-32826 — The importance of organic molecules with large two-photon absorption (2PA) is realized for deep-tissue fluorescence microscopy, photodynamic therapy, three-dimensional microfabrication and optical data storage. Computer predictions provide understanding of structure/activity relationships and assist in the rational design of polymer materials as an alternative to trial and error methods. In this contribution, we compare various density functional theory (DFT) formalisms to predict two-photon absorption spectra in a series of large donor-acceptor substituted conjugated molecules. We conclude that the accuracy of a posteriori Tamm-Dancoff approximation [1] is close to the exact results obtained in Coupled Electronic Oscillators formalism [2]. Adjusting fraction of exact exchange in XC functionals allow for improved agreement with experiment. [1] Mikhailov, I.A.; Tafur, S.; Masunov, A.E., Phys. Rev. A 77, 01250 (2008) [2] Masunov, A.M.; Tretiak, S., J. Phys. Chem. B 108, 899 (2004)

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