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Dynamical Hyperpolarizabilities from Real-Time Density Functional Theory VLADIMIR GONCHAROV, KALMAN VARGA, Vanderbilt University — The explicitly time dependent wave function obtained in the framework of Real-Space, Time-Dependent Density Functional Theory captures the essential physics and allows a non-perturbative calculations of important observables. We generalize finite-difference method typically used to calculate static hyperpolarizabilities to the dynamical case [1] and compute nonlinear optical response functions to the third order inclusively. The method is simple and free of errors associated with basis function based methods. Comparison with experimental results for a range of molecules including C_{60} is presented.

[1]V. A. Goncharov and K. Varga, *J. Chem. Phys.*, 2012, 137, 094111

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