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Linear and Non-Linear Optical Response using Real-Time Time-Dependent Density Functional Theory[1] Y. TAKIMOTO, F.D. VILA, J.J. REHR, Univ of Washington — We present an approach for the calculation of the frequency- dependent response of nano-scale organic molecules for non-linear optical (NLO) devices. These calculations are performed using an efficient implementation of real-time, time-dependent density functional theory (RT-TDDFT) [2], and an adaptation of the SIESTA electronic structure code. This method yields frequency dependent nonlinear optical properties of large organic molecules, which have been difficult to obtain with frequency domain calculations. Here we discuss the efficiency of the method and compare the results against frequency-domain TDDFT methods and with experiment. Solvent effects on the NLO properties of photonic molecules are also briefly discussed.

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[2]Y. Takimoto, F. D. Vila, and J. J. Rehr, J. Chem. Phys. **127**, 154114 (2007)

Yoshinari Takimoto
Univ of Washington

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