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Real space, real time approach for linear and non-linear optical response of nano-scale molecules[1] YOSHINARI TAKIMOTO, FERNANDO VILA, JOHN REHR, University of Washington — We present a real time, time-dependent density-functional theory approach for the calculation of the frequency-dependent optical responses, which is based on the approach of Tsolakidis et al. [1] This approach is extended for the calculation of non-linear response. Tensor components of linear polarizabilities and first order hyper-polarizabilities are extracted by fitting the net time dependent polarization with different electric field strengths. This real-space, real-time method is computationally efficient and generic in that it requires no symmetry assumptions. Results are presented for several organic molecules, e.g., FTC and PNA, including both linear and nonlinear response. [1] A. Tsolakidis, D. Sanchez-Portal and R.M. Martin, Phys. Rev. B **66**, 235416 (2002).

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