Real time approach for non-linear optical response of nano-scale systems\textsuperscript{1} Y. TAKIMOTO, F. VILA, J.J. REHR, U. of Washington — We present a real-time, time-dependent density-functional approach for the calculation of the frequency-dependent linear and non-linear optical response, which is based on the approach of Tsolakidis et al.\textsuperscript{2} Tensor components of linear polarizabilities and first order hyper-polarizabilities are extracted by fitting net time dependent polarizations with different electric field strengths. The method is computationally efficient and can be applied to large, molecular and nano-scale systems. Results are presented for C\textsubscript{60} and for a number of “push-pull” molecules. Our results for the static limit are in good agreement with other density-functional calculations.

\textsuperscript{1}Supported by NSF Grant DMR-0120967 (Y.T. and F.V) and DOE Grant DE-FG02-97ER45623 (JJR) and facilitated by the DOE CMSN

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Date submitted: 04 Dec 2005

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