

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Real time approach for non-linear optical response of nano-scale systems¹ 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.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 C₆₀ and for a number of “push-pull” molecules. Our results for the static limit are in good agreement with other density-functional calculations.

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

²A. Tsolakidis, D. Sanchez-Portal and R.M. Martin, Phys. Rev. B **66**, 235416 (2002).

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Date submitted: 04 Dec 2005

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