Abstract Submitted
for the MAR05 Meeting of
The American Physical Society

Theoretical Calculations of Nonlinear Optical Response[1] F. VILA, Y. TAKIMOTO, J.J. REHR, U. of Washington — Nonlinear optical (NLO) devices play a key role in many applications. A systematic approach for the design and synthesis of materials with desirable NLO properties has been difficult to achieve, and hence theoretical methods are desirable. Usually systems with sizable NLO properties are large, limiting the theoretical methods that can be used. Here we examine two approaches for calculating the polarizabilities and first hyperpolarizabilities of large systems. First, we discuss the applicability of density functional theory (DFT), with special attention to difficulties of applying it in systems where non-locality can be important. Results are presented for "push-pull" molecules, which have some of the largest hyperpolarizabilities reported to date. Second, we present a self-consistent real space multiple scattering approach for calculating both linear and nonlinear response of large systems. The approach is illustrated with sample calculations including C60 and other large molecules.

[1]Supported in part by NSF grant DMR0120967

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Date submitted: 22 Dec 2004 Electronic form version 1.4