Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Ab Initio **Study of Atomic and Molecular Polarizabi-lities**[1] IGOR VASILIEV, New Mexico State University, JAMES R. CHELIKOWSKY, The University of Texas at Austin — We calculate the static electric dipole polarizabilities for a variety of atoms and molecules using a finite field method implemented in the framework of an *ab initio* density functional formalism. Our calculations employ several different representations of the exchange-correlation potential, including the local density approximation, generalized gradient approximation, and asymptotically correct functionals introduced by Leeuwen-Baerends [1] and Casida-Salahub [2]. We observe that the computed values of polarizabilities are strongly influenced by the asymptotic behavior of the density functional exchange-correlation potential. The accuracy of theoretical atomic and molecular polarizabilities is substantially improved by the use of asymptotically correct exchange-correlation functionals. This result can be explained in terms of electronic excitation energies and the polarizability sum rule.
[1] R. van Leeuwen and E. J. Baerends, Phys. Rev. A 49, 2421 (1994).
[2] M. E. Casida and D. R. Salahub, J. Chem. Phys. 113, 8918 (2000).

[1]This work was supported in part by NSF under DMR-0551195, ACS under PRF-48556-AC10, and the U.S. Department of Energy under DE-FG36-08GO88008, DE-FG02-06ER46286, and DE-FG02-06ER15760.

Igor Vasiliev
New Mexico State University

Date submitted: 23 Nov 2008 Electronic form version 1.4