

Static dipole polarizabilities through density functional methods

Fuentealba, P.

Simón-Manso, Y.

Various density functionals have been tested in calculating atomic and molecular dipole polarizabilities. For atoms, it has been found that the results are not competitive with more sophisticated ab initio methods. Exchange and correlation effects have been analyzed separately to show that the main cause of errors lies in the exchange functional models. Strong numerical evidence is given to support the idea that a right asymptotic behavior of the exchange potential is essential to obtain reliable values for the dipole polarizabilities. In this sense, the hybrid method proposed by Becke (J. Chem. Phys. 1993, 98, 5648) and the phenomenological exchange potential proposed by van Leeuwen and Baerends (Phys. Rev. 1994, A49, 2421), performed much better. For molecules, the comparison is more difficult because of the scarcity of reliable experimental values as well as ab initio calculations including correlation effects. The results have however shown that the bonding effects predominate over