Russian Journal of General Chemistry 1998 vol.68 N11, pages 1808-1812

Electronegativity in the Density Functional Theory. Determination of the Electron Chemical Potential of the Ground State of a System in the Local Density Approximation

Zueva E., Galkin V., Cherkasov A., Cherkasov R.
Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia

Abstract

An iterative algorithm for simultaneous determination of the ground-state electron chemical potential and electron density of a multielectron system is formulated in terms of the density functional theory. With the energy potential in the local density approximation as an example it is shown that the equality of the electronegativities of the natural orbitals corresponds to the nonphysical electron density.