

A modified version of the electron localization function (ELF)

Fuentealba,

Using some relationships derived from the density functional version of the virial theorem, an approximated kinetic energy density is constructed. This is used to implement a modified version of the electron localization function (ELF). Its principal differences with the original ELF are that it does not depend on the orbitals and it reduces to zero when the distance r to the nucleus goes to 0 or infinity. Otherwise, it reproduces all the properties of the ELF function. However, the conceptual interpretation of ELF as coming from the pair probability is lost. © 1998 John Wiley & Sons, Inc.