龙讯教程

Electron localization function（ELF）

support@pwmat.com

Introduction

In quantum chemistry, the electron localization function (ELF) is a measure of the likelihood of finding an electron in the neighborhood space of a reference electron located at a given point and with the same spin. Physically, this measures the extent of spatial localization of the reference electron and provides a method for the mapping of electron pair probability in multielectronic systems.

ELF's usefulness stems from the observation that it allows electron localization to be analyzed in a chemically intuitive way. For example, the shell structure of heavy atoms is obvious when plotting ELF against the radial distance from the nucleus; the ELF for radon, for example, has six clear maxima, whereas the electronic density decreases monotonically and the radially weighted density fails to show all shells. When applied to molecules, an analysis of the ELF shows a clear separation between the core and valence electron, and also shows covalent bonds and lone pairs, in what has been called "a faithful visualization of VSEPR theory in action". Another feature of the ELF is that it is invariant concerning the transformation of the molecular orbitals.

The ELF was originally defined by Becke and Edgecombe in 1990.[1] They first argued that a measure of the electron localization is provided by

$$D_\sigma(\mathbf{r}) = \tau_\sigma(\mathbf{r}) - \frac{1}{4}\frac{(\nabla\rho_\sigma(\mathbf{r}))^2}{\rho_\sigma(\mathbf{r})},$$

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where ρ is the electron spin density and τ the kinetic energy density. The second term (negative term) is the bosonic kinetic energy density, so D is the contribution due to fermions. D is expected to be small in those regions of space where localized electrons are to be found. Given the arbitrariness of the magnitude of the localization measure provided by D, it is compared to the corresponding value for a uniform electron gas with spin density equal to ρ(r), which is given by

$$D_\sigma^0(\mathbf{r}) = \tfrac{3}{5}(6\pi^2)^{2/3}\rho_\sigma^{5/3}(\mathbf{r}).$$

The ratio, $$\chi_\sigma(\mathbf{r}) = \frac{D_\sigma(\mathbf{r})}{D_\sigma^0(\mathbf{r})},$$

is a dimensionless localization index that expresses electron localization for the uniform electron gas. In the final step, the ELF is defined in terms of χ by mapping its values on to the range 0 ⩽ ELF ⩽ 1 by defining the electron localization function as

$$\mathbf{ELF}(\mathbf{r}) = \frac{1}{1+\chi_\sigma^2(\mathbf{r})}.$$

ELF = 1 corresponding to perfect localization and ELF = ½ corresponding to the electron gas.

1. A. D. Becke and K. E. Edgecombe (1990). "A simple measure of electron localization in atomic and molecular systems". J. Chem. Phys. 92 (9): 5397–5403. Bibcode:1990JChPh..92.5397B. doi:10.1063/1.458517.

Example：

Notice： please update PWmat version later than 20210221

Set out.elf = t in etot.input， it will output OUT.ELF file， U can convert it to xsf formate by using convert_rho.x utility and open the new xsf file with VESTA

```
1   4
in.atom=atom.config
job = scf
in.psp1 = Cu.SG15.PBE.UPF
ecut = 70
ecut2 = 280
mp_n123 = 12 12 12 0 0 0
out.elf = t
```

It is sensitive to ecut, for get better results, set ecut2=4ecut

Example

convert_rho.x OUT.ELF , open the new RHO.xsf file with VESTA