MULTIWFN

A Multifunctional wavefunction analyzer

Tian Lu
Department of Chemistry and Chemical Engineering, School of Chemical and Biological Engineering,
University of Science and Technology Beijing, Beijing 100083

Overview

Multiwfn is a free, flexible, powerful wavefunction analysis program, based on Windows and Linux platform, its main functions include:

- Viewing molecular structure and orbitals
- Calculating value at a point, in a line, in a plane or in a spatial scope for many real space functions
- Population analysis
- Bond order analysis
- Orbital composition analysis
- Topology analysis for real space functions
- Plotting density-of-state and spectrum
- Quantitative molecular surface analysis
- Viewing and processing Gaussian-type cube files
- Many utilities involved in quantum chemistry analyses

Supported real space functions

- Electron density and its gradient norm as well as Laplacian
- Spin density
- Hamiltonian / Lagrangian kinetic energy density
- Electrostatic potential from electrons or nuclei
- Electron localization function
- Localized orbital locator
- Local information entropy
- Reduced density gradient
- Sign(λ_2)*ρ
- Fermi hole / correlation factor function
- Average local ionization energy

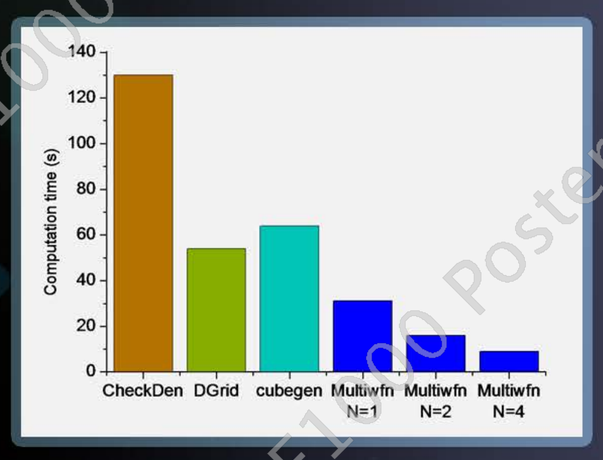
Special points

► Very user-friendly

Multiwfn is designed as an interactive and semi-GUI program, there is no any barrier even for beginners. About thirty detailed tutorials are given in the manual for helping users to learn the usage.

► No third-part plotting softwares are required

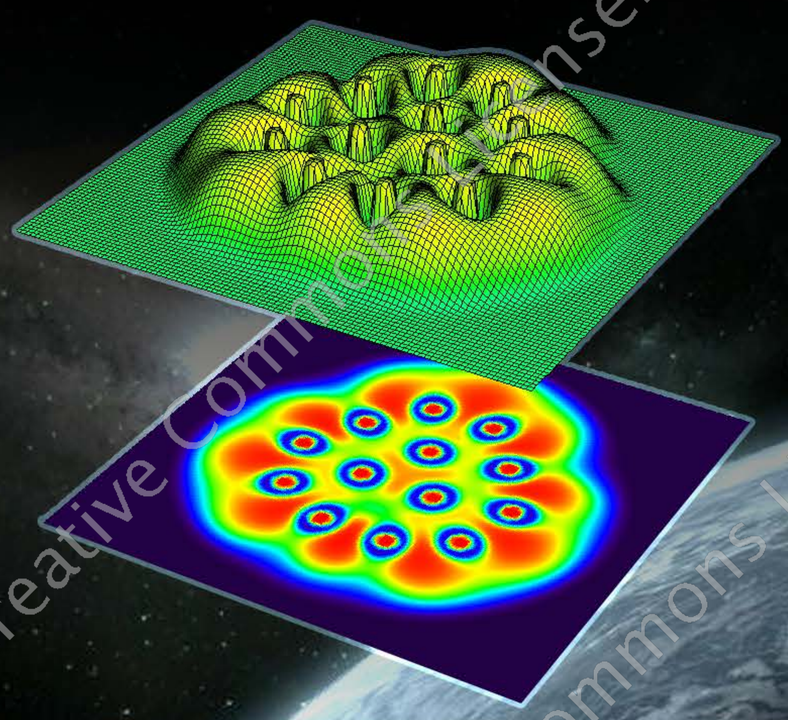
Multiwfn has a built-in graphical module for directly visualizing results, thus the procedure of wavefunction analysis is remarkably simplified.



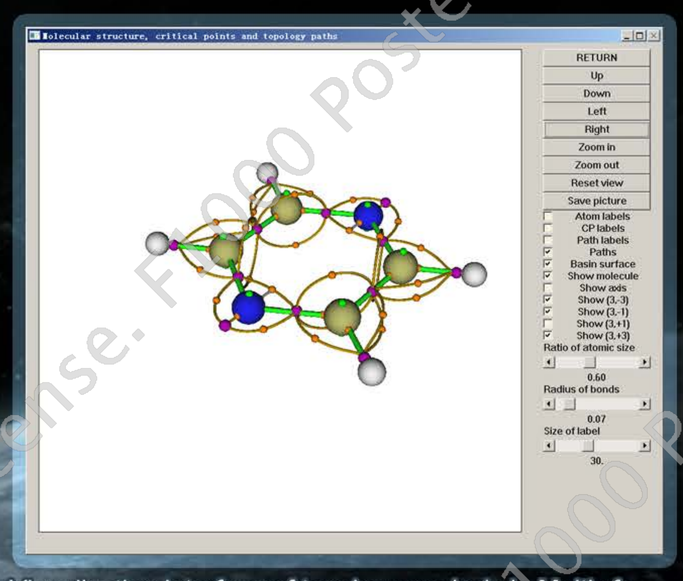
► High efficiency

The code of Multiwfn has been substantially optimized. Most time-consuming calculations have been parallelized. The efficiency is evidently higher than related softwares.

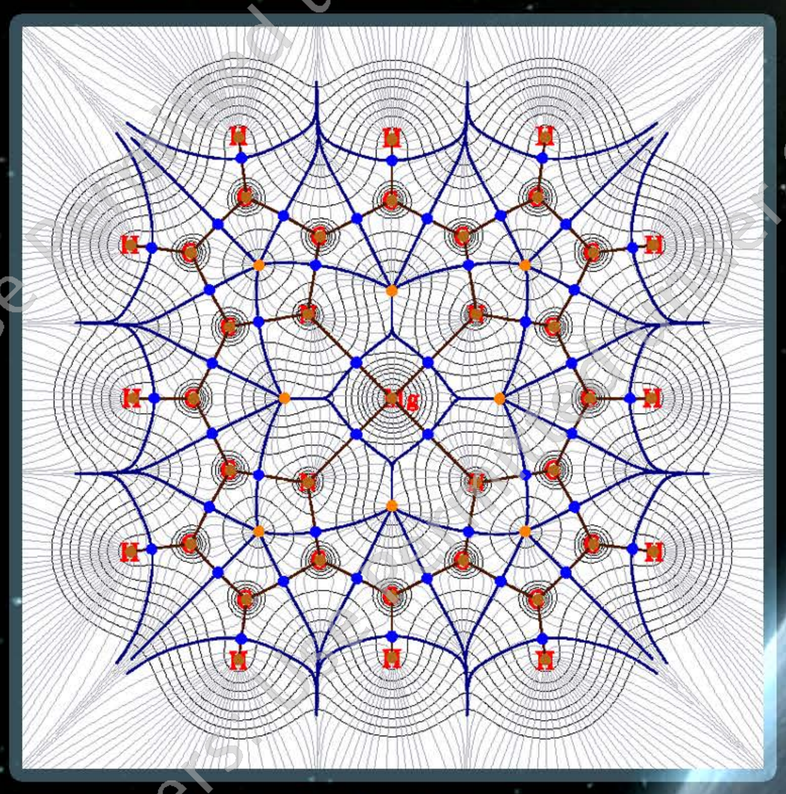
Time spent in generating grid data of electron density Laplacian for acetic acid 6-31G** basis-set, 623392 points in total, tested on Intel i7-2630QM CPU. *N* denotes the number of threads



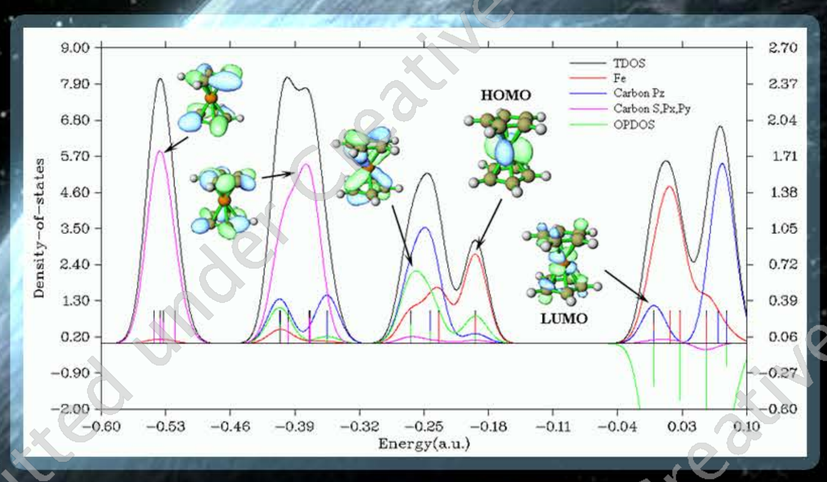
Electron localization function map of B_{13}^+ cluster



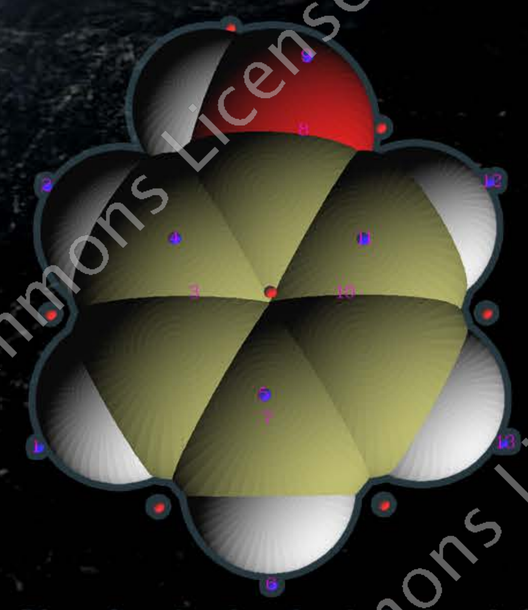
Visualization interface of topology analysis in Multiwfn. Critical points and corresponding paths of localized orbital locator of pyrazine are shown



Gradient map of electron density with contour lines of magnesium porphyrin. Critical points, bond paths, interbasin paths are also shown



Total / Partial / Overlap density-of-state (DOS) map of ferrocene. Orbital isosurfaces rendered by Multiwfn are also appended on



Minima (blue spheres) and maxima (red spheres) of average local ionization energy on van der Waals surface of phenol

For details please visit: **http://Multiwfn.codeplex.com**