**\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\*\* autoCDFT**

**- A Python tool for an automated conceptual DFT analysis –**

**Software Manual**

**v 1.2 (dev)**

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**website:** [**http://github.com/javialra97/autoCDFT**](http://github.com/javialra97/autoCDFT)

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**1.1 Files of autoCDFT**

autoCDFT.py: The executable file.

information.txt: The parameters to run *autoCDFT*.

**1.2 Input files**

*name.out*: This file is the output of Gaussian software, the calculation should be a single point.

*\*\*\*.chg*: This file is the output of Multiwfn software, the calculation should be population analysis. The name must be distinguished by the word *cation*, *anion* o *neutro*. It is not neccesary the calculation just the formatted.

*information.txt*: In the first and second column you should write *name.out* of each pair. In the last two columns you should write first how many atoms you want to analyze, follow by ‘-’ and then the number of the atom(s) and ‘-’ again.

**1.3 Output files**

For each pair you will obtain a txt file that contain the corresponding information to the frontier molecular orbitals, the global and local descriptors. The latter over the atoms that it was especified in *information.txt.* Also you will obtain an *excel* file called name\_summary.xlsx where you will find all the information to compound .

You should have the *openpyxl* library installed.