Charge Transfer Unveiled: An Exciting Journey Through TD-DFT

Case-study Walkthrough

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Gaussian is proprietary software.

Software to be used (pre-installed on *Aristotle*)

1) Gaussian 16

2) **GaussView**

3) GaussSum

Software to install on local machine

1) Notepad++ (or any other text editor) (Windows specific)

https://notepad-plus-plus.org/downloads/

Download: Notepad++ 8.7.1 release

ORCA and **Gaussian** are proprietary software.
ORCA is distributed free for academic use.

Download the following software

1) ORCA 6

https://orcaforum.kofo.mpg.de/index.php

Downloads -> ORCA 6.0.1
choose depending on your system

2) **GaussView** – Avogadro (ORCA enhanced version)

https://orcaforum.kofo.mpg.de/index.php

Downloads -> Avogadro (ORCA enhanced version)
choose depending on your system
Warning. New version supports ORCA 6 but is beta.

3) Notepad++ (or any other text editor) (Windows specific)

https://notepad-plus-plus.org/downloads/

Download: Notepad++ 8.7.1 release

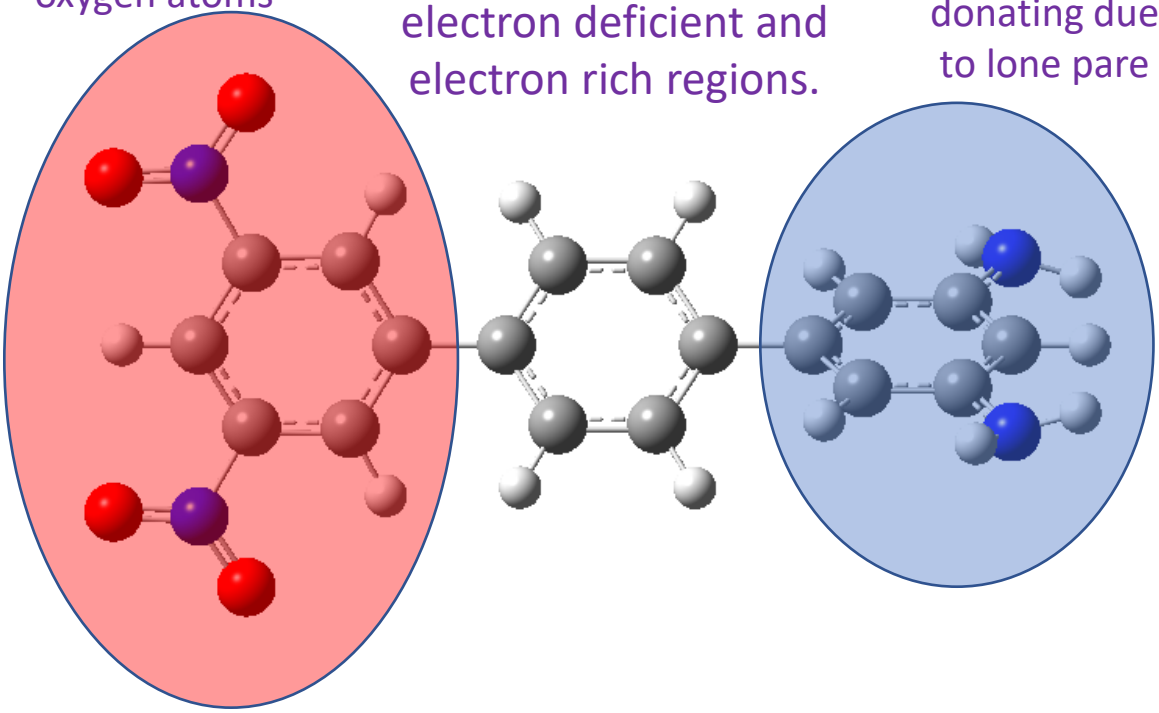
Let's **design** a molecule that we (really!) expect to exhibit some CT upon excitation.

The molecule should have at least two groups/regions with very different electron availability.

$-NO_2$ electron withdrawing due highly electronegative oxygen atoms

Bridging group. Increase distance between electron deficient and electron rich regions.

$-NH_2$ electron donating due to lone pare



Electron Poor region containing $-NO_2$

Electron Rich region containing $-NH_2$

Let's build the molecule using GaussView!

Cubes file general format

Taken from our run.

```
NO2-benzene--benzidine excited state 23 @ M06/D2SVP
mo=90
 MO coefficients
   40  -16.330340  -11.400123   -9.410322    1
  107    0.333333    0.000000    0.000000
   69    0.000000    0.333333    0.000000
   57    0.000000    0.000000    0.333333
    6    6.000000    7.241708   -0.000004    0.000000
    6    6.000000    8.560333   -1.146586    1.980913
…
  6.06724E-17  1.24724E-16  2.45869E-16  4.62439E-16  8.23051E-16  1.36619E-15
  2.05476E-15  2.61041E-15  2.14718E-15 -1.55637E-15 -1.33607E-14 -4.28444E-14
 -1.07169E-13 -2.34245E-13 -4.64875E-13 -8.51576E-13 -1.45126E-12 -2.30981E-12
 -3.43958E-12 -4.79543E-12 -6.25967E-12 -7.64700E-12 -8.73598E-12 -9.32250E-12
…
  1.31347E-16  2.69058E-16  5.27387E-16  9.82465E-16  1.71902E-15  2.76153E-15
  3.86878E-15  4.02062E-15  2.77480E-16 -1.45109E-14 -5.58608E-14 -1.54360E-13
 -3.65004E-13 -7.77598E-13 -1.52387E-12 -2.77359E-12 -4.71034E-12 -7.48032E-12
 -1.11178E-11 -1.54662E-11 -2.01302E-11 -2.44950E-11 -2.78350E-11 -2.94946E-11
…
```

Interactively run **cubegen** preferably via GaussView:

```
cubegen <filename>.fchk
```

Detailed information are provided at:
https://gaussian.com/cubegen/
http://paulbourke.net/dataformats/cube/