Orbitals: Population Analysis, Transformation and Visualization

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Contents

Wavefunction-based Atomic Charges

- Mulliken charges, Löwdin charges
- NPA charges
  `pop=nbo`

Real-space-based Atomic Charges

- Hirshfeld charges
- Becke charges
- AIM charges

Electrostatic-potential-based Atomic Charges

- MK
- CHelpG

NBO Technical Details

Run NBO3.1 via Gaussian

```
#p B3LYP/6-31G(d,p) Pop=NBORead

Example of NBO bond orders

0  1
C     0.000000    0.665676    0.000000
H     0.919278    1.237739    0.000000

$nbo $end
```
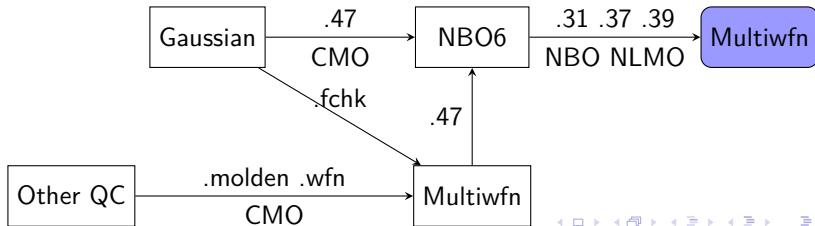
Run NBO6/7

```
$nbo archive file=... $end
```

Useful NBO keywords

- $NBO NLMO PLOT $END
- user-defined search.
    - NBO6

```
$CHOOSE
BOND S 1 28
     S 1 29 END
3CBOND S 1 28 29 END
$END
```

    - NBO7
      $NBO MOLUNIT <1,28,29> $END

Orbital Localization