Natural orbitals and natural transition orbitals

1. Read 2 NTO papers and relevant section from Q-Chem manual (everyone should read both papers!)
2. Revisit CIS calculations of formaldehyde and perform NTO analysis of the excited states.
3. On October 4, we will discuss these concepts in the following order:
   - Sahil will present Paper 1/manual: Theory of NTO and different exciton properties computed by libwfa (participation ratio, $<r_e>$ versus $<r_h>$, etc.).
   - Ariel will present selected examples from Paper 2
   - Bibek will present NTOs for formaldehyde and NTOs for his molecule, with exciton properties analysis

Each presentation is 20 min.

Practical considerations:
To compute NTOs and NOs, add the following to the CIS (or other excited-state job) input:

```
$rem
   state_analysis true
   molden_format true
   ntopairs 3
$end
```

Once the job is complete, use Gabedit or Jmol to visualize NO and NTOs which are in the xxx.plots directory. The former is more powerful, but the latter is simpler to master.