

## Building the system

Import xyz-  
coordinates

Visualize,  
distances, ...

SMILES  
string

Optimize  
structure

## Optimizing the electronic structure

Self-consistent  
field (SCF)

Visualize MOs,  
energies, ...

MCSCF / post-HF

## Spectrum calculation

UV/vis

...

XAS

## Spectrum analysis

Energy, intensity,  
polarization,  
dominant  
amplitudes...

NTOs

Plot spectra

