



# Overview :

## Molden

- Draw molecule

## GAMESS

- Quantum chemistry
- Optimize geometry

## Huckel-IV

- I-V calculation

The screenshot shows the NanoHUB website interface. At the top, the logo "nanoHUB" is displayed in a stylized font. Below the logo, it states "Operated by the Purdue Computational Electronics Research Group" and "The Nanotechnology Simulation Hub Online Computing for Nanotechnology". The navigation bar includes "HOME", "MY HUB", and "HUB FORUMS". The main content area is divided into three columns: "NANOTOOLS", "CHEMISTRY", and "DEVICES".

**NANOTOOLS**

- NANO/MOLECULAR
  - [CNTbands](#)
  - [FETToy](#)
  - [Huckel-IV 2.0](#)
  - [MolCToy](#)
  - [NanoMOS 2.5](#)
  - [Schred](#)
  - [IBGreen](#)
  - [TunProb](#)
- MATERIALS
  - [MOSCV](#)

**CHEMISTRY**

- [ABINIT](#) NEW!
- [CPMD](#) NEW!
- [GAMESS](#)
- [Molden](#)
- [RasMol](#) NEW!
- [VMD/NAMD](#) (offsite)

**ECAD**

- [Spice3f4](#)
- [Spice2G](#)
- [VLSOL/Spice2](#)

**DEVICES**

- [Adept](#)
- [Demon](#)
- [Medici](#)
- [Minimos](#)
- [SDemon](#)
- [Sequal](#)

**PROCESS**

- [Prophet](#)
- [TSuprem4](#)
- [ThermoEMP](#)

Arrows from the text on the left point to the following links in the screenshot:

- Molden points to the [Molden](#) link in the CHEMISTRY column.
- GAMESS points to the [GAMESS](#) link in the CHEMISTRY column.
- Huckel-IV points to the [Huckel-IV 2.0](#) link in the NANOTOOLS column.

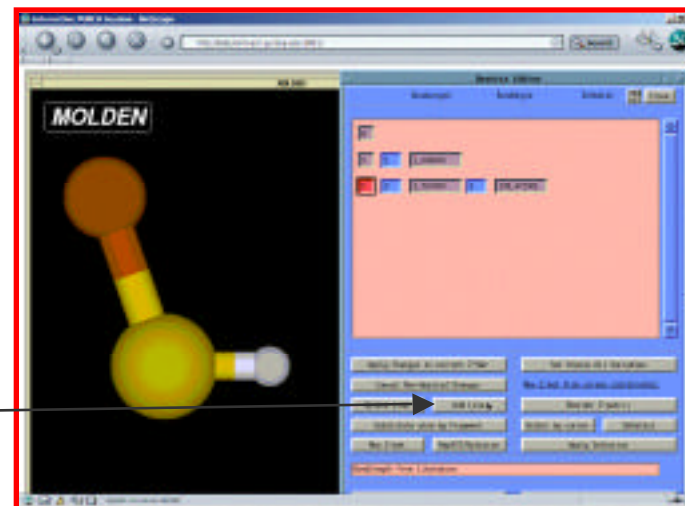
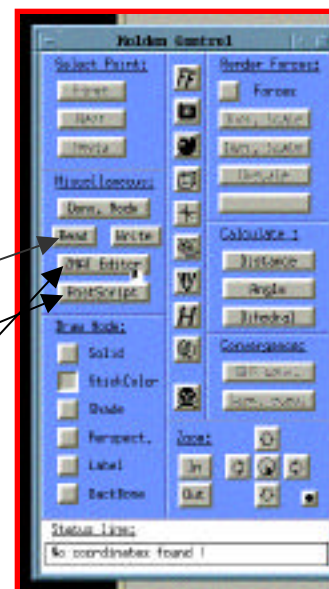
# Molden : Drawing the molecule

## ■ Molden

- ❑ Read and write several different formats
- ❑ Generate "pretty" pictures (postscript)
- ❑ Define molecule using z-matrix editor

## ■ New molecule

- ❑ Open z-mat editor
- ❑ Add atoms etc....



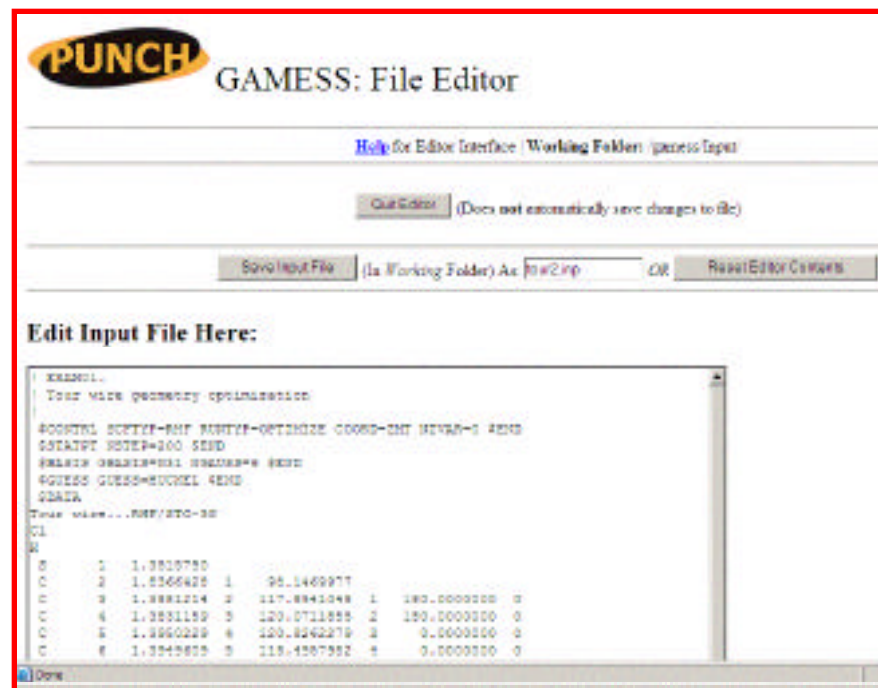
# GAMESS : Optimize geometry

## ■ Input file

- ❑ Copy z-matrix from Molden file
- ❑ Choose method and basis set
- ❑ Simple basis set first, then improve with better basis set
- ❑ Example on the nanoHub

## ■ Output file

- ❑ Check for convergence



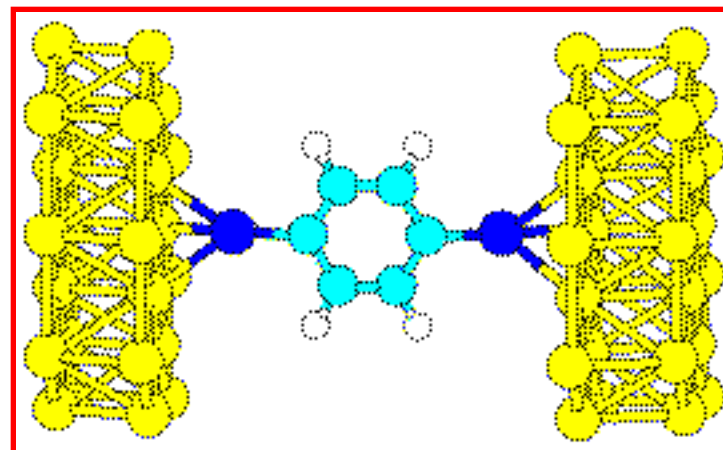
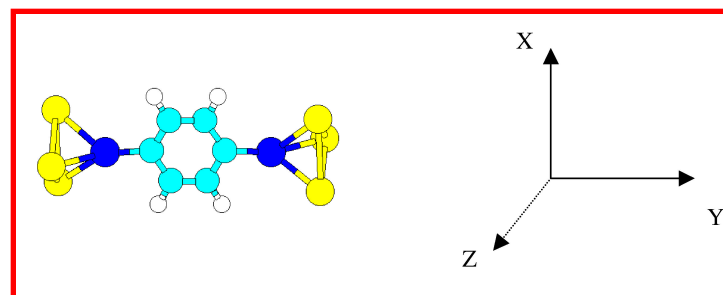
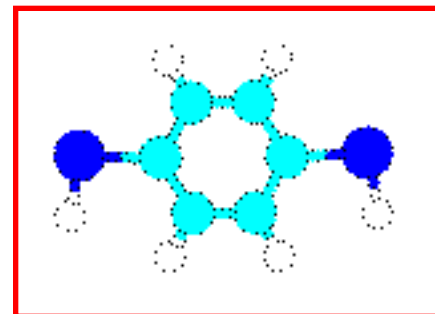
The screenshot shows the PUNCH GAMESS: File Editor interface. The title bar reads "PUNCH GAMESS: File Editor". Below the title bar, there is a "Help for Editor Interface" link and a "Working Folder" field containing "game32.inp". A "Quit Editor" button is present with the tooltip "(Does not automatically save changes to file)". Below that, there is a "Save Input File" button, a "Working Folder" field containing "game32.inp", and a "Reset Editor Contents" button. The main area is titled "Edit Input File Here:" and contains a text editor window with the following input file content:

```
*****
! Test with geometry optimization
$CONFIG SCFTYP=RMF RUNTYP=OPTIMIZE COORD=INT NITER=3 #END
$STATPT SCFEP=100 #END
$HEATP SCHEM=HLL SCHEM=HLL #END
$GUESS GUESS=HUCKEL #END
$DATA
Title: test...RHF/STO-3G
CL
M
O      1  1.3510750
C      2  1.8266425  1  95.1469977
C      3  1.8881214  2  117.8841048  1  180.0000000  0
C      4  1.3531189  3  120.0711885  2  150.0000000  0
C      5  1.8560229  4  120.8242279  3  0.0000000  0
C      6  1.3545655  5  115.4267582  4  0.0000000  0
```

# Huckel-IV :

## Input geometry

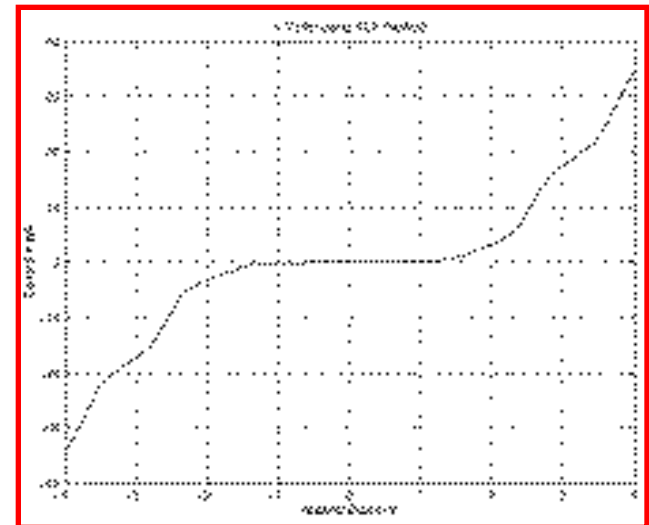
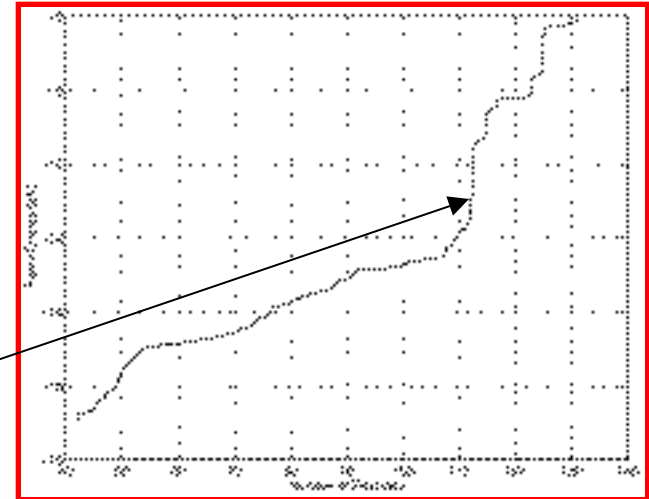
- Huckel-IV needs
  - Geometry
  - Fermi energy
  - Charging energy
- Input geometry
  - Cut and paste molecular coordinates from GAMESS (Cartesian format)
  - Run Matlab script on nanoHub to rotate molecule



# Huckel-IV :

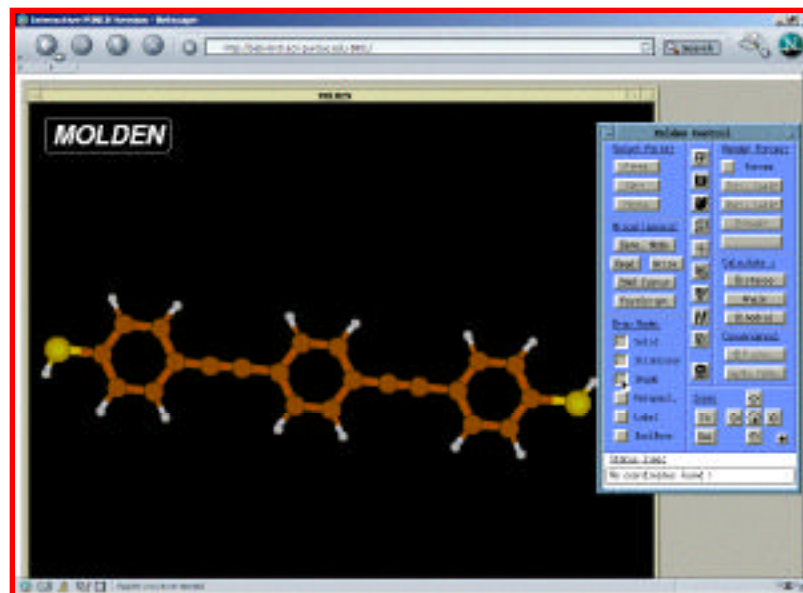
## Fermi energy

- **Determine Fermi-level**
  - ❑ Extended Huckel theory cannot estimate the Fermi energy
  - ❑ Charge neutrality level
  - ❑ Fermi energy for gold contact is -9.5 eV (Huckel)
  - ❑ Fermi energy between these two values (-11 eV)
- **Charging energy (U)**
  - ❑ PDT 1-2 eV
  - ❑ Larger molecules \_ smaller U



# Summary :

- Molden
- GAMESS
- Huckel-IV



- New version of Huckel-IV
  - Faster and proper electrostatics (including a gate)
  - Expected to be ready this autumn