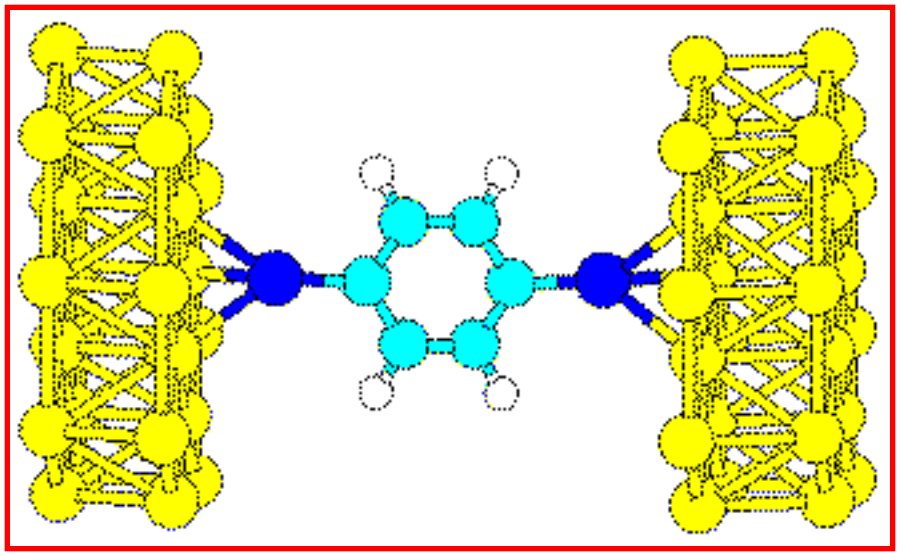
Huckel-IV on the nanoHub

M. Paulsson, F. Zahid and S. Datta

MolCToy

Huckel-IV 2.0

- Geometry of molecule
- Contacts
- Fermi energy
- Charging energy



Overview :

Molden

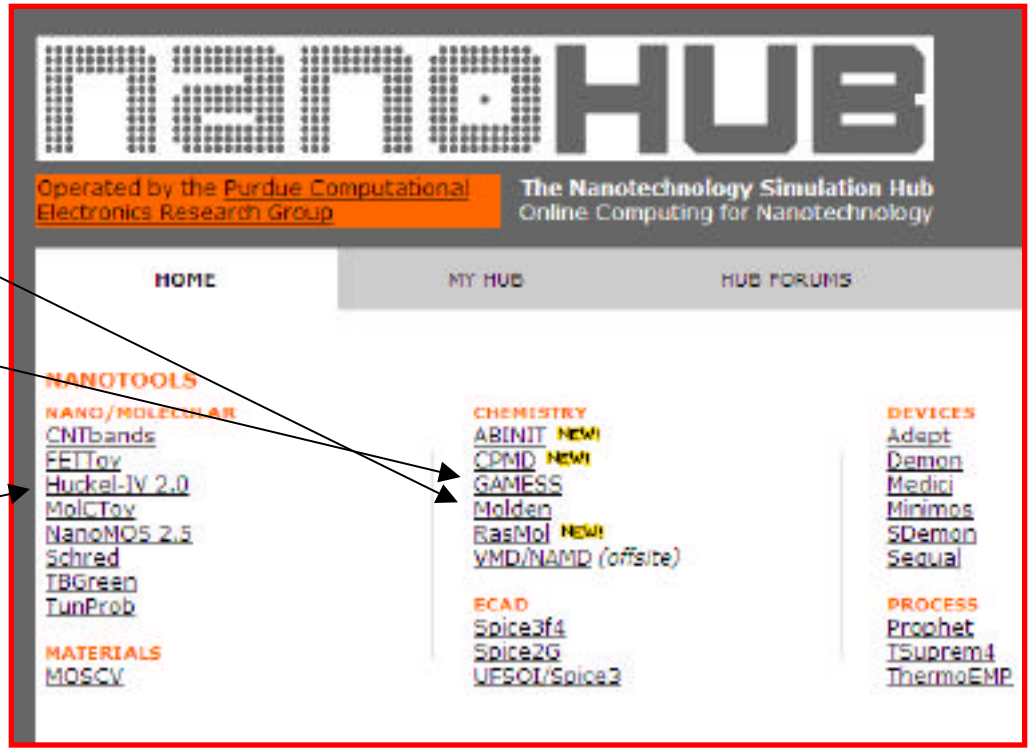
- Draw molecule

GAMESS

- Quantum chemistry
- Optimize geometry

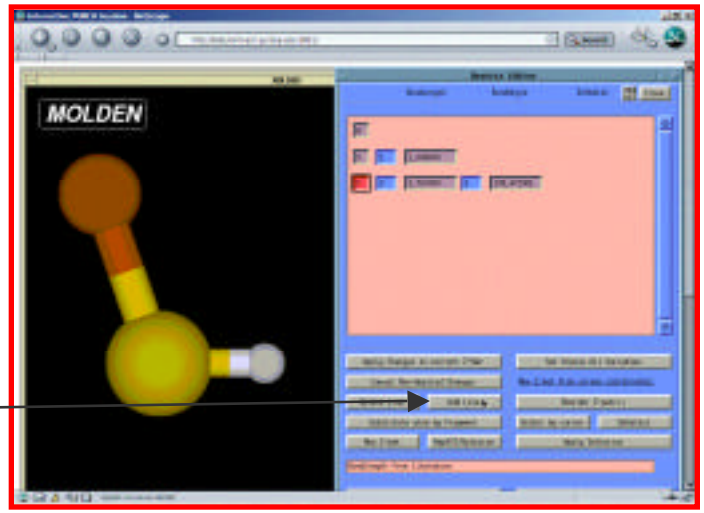
Huckel-IV

- I-V calculation



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….

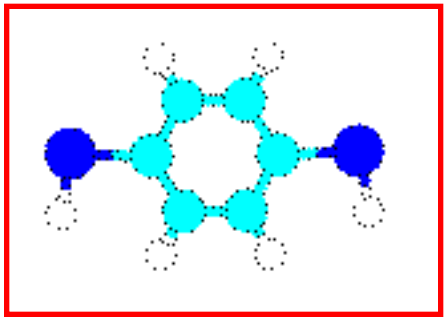


GAMESS : Optimize geometry

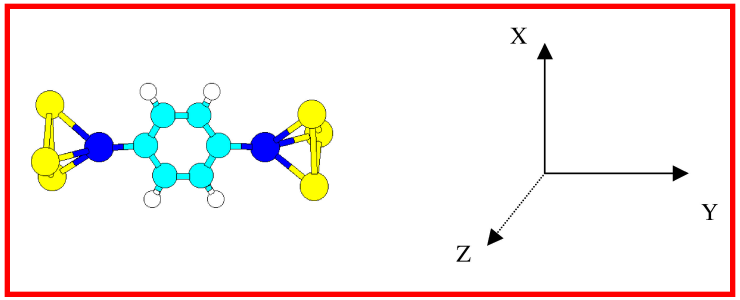
- **Input file**
  - Copy z-matrix from Molden file
  - Choose method and basis set
  - Simple basis set first, then improve with better basis set
  - Example on the nanoHub
- **Output file**
  - Check for convergence

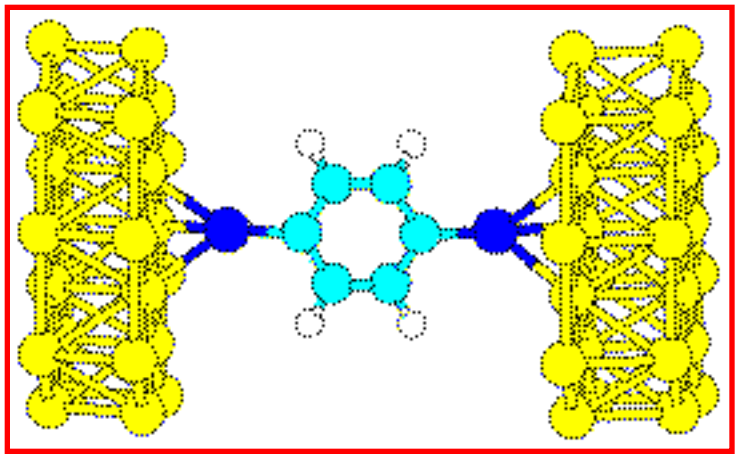
GAMESS, maintained by Gordons research group, Iowa State University.

Huckel-IV : Input geometry



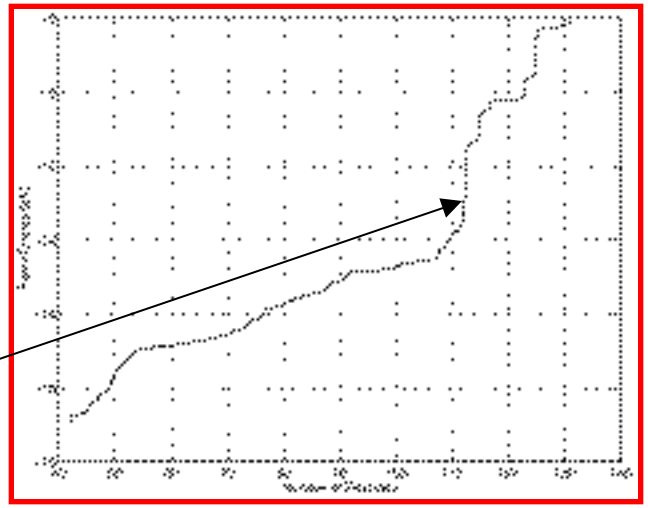
- **Huckel-IV needs**
  - Geometry
  - Fermi energy
  - Charging energy
- **Input geometry**
  - Cut and paste molecular coordinates from GAMESS (Cartesian format)
  - Run Matlab script on nanoHub to rotate molecule

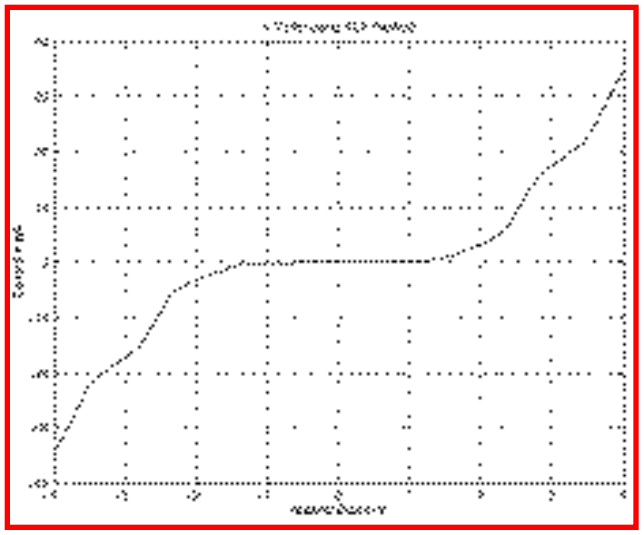




Huckel-IV : Fermi energy

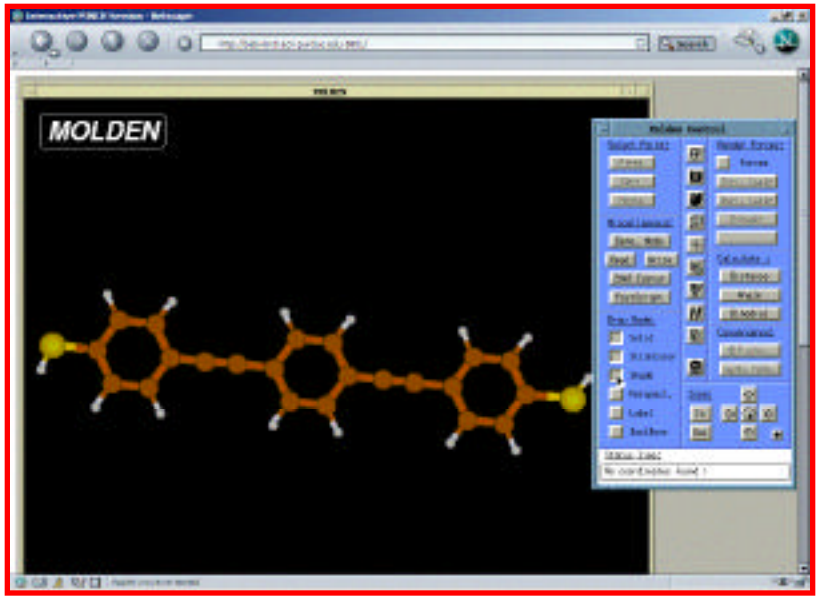
- **Determine Fermi-level**
  - Extended Huckel theory cannot estimate the Fermi energy
  - Charge neutrality level
  - Fermi energy for gold contact is -9.5 eV (Huckel)
  - Fermi energy between these two values (-11 eV)
- **Charging energy (U)**
  - PDT 1-2 eV
  - Larger molecules _ smaller U





Summary :

- **Molden**
- **GAMESS**
- **Huckel-IV**



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