What can you do with Gaussian09 on Turing?

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www.gaussian.com
What is Gaussian09?

- Electronic structure software package
- Introduced by Nobel Laureate John Pople in 1970
- Approximate solutions to Schrödinger’s Equation
  \[ H\psi = E\psi \]

- Applications:
  - Optimizing geometries of chemical structures
  - Calculating chemical properties (IR, NMR, UV/Vis, etc)
  - Modeling reaction mechanisms
Running G09 jobs

- What do you need to run a G09 job?
  - Structure
  - Basis set – represents the wavefunction
  - Method – represents the Hamiltonian
    - Inexpensive, but inaccurate (MM, semiempirical)
    - Expensive, state-of-the-art (CCSD(T))
    - Balanced (DFT, current favorite)
      - Wide range of functionals available
      - Fast on multiprocessor execution

- GaussView – GUI

Lewisite/British Anti–Lewisite


Selected Publications from HPC resources


\( \pi-\pi \) stacking interactions

- Important non-bonding interaction
  - Petroleum science, nanotubes
  - Biochemical recognition
  - Crystal packing

- We are developing new models
- Turing allows us to handle larger systems
Healthy thyroid function requires Iodine and selenium!

Mechanism known, but how does it occur?
- Protein structure was unknown until recently

Important to treat thyroid illnesses

Our novel mechanism modeled with G09 with small models

Verified in prestige journals (JACS and PNAS)

Scale up with Turing!
Modeling with Turing

Pre-Turing

Turing

And Beyond…
Pigments extracted from *Stentor* are photosensitive and potential photodynamic therapy agents

- Compounds are difficult to characterize
- Simulation of the UV/Vis spectrum using TD–DFT
- Model mechanisms