Physical Chemistry II: Quantum Chemistry
Lecture 21: WebMO Demo

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Computational Chemistry Methods

- Molecular mechanics
- Semiempirical molecular orbital methods
- *Ab initio* molecular orbital methods
- Density functional method
- Quantum Monte Carlo method
- …

Yields Energy, Structure, and Properties

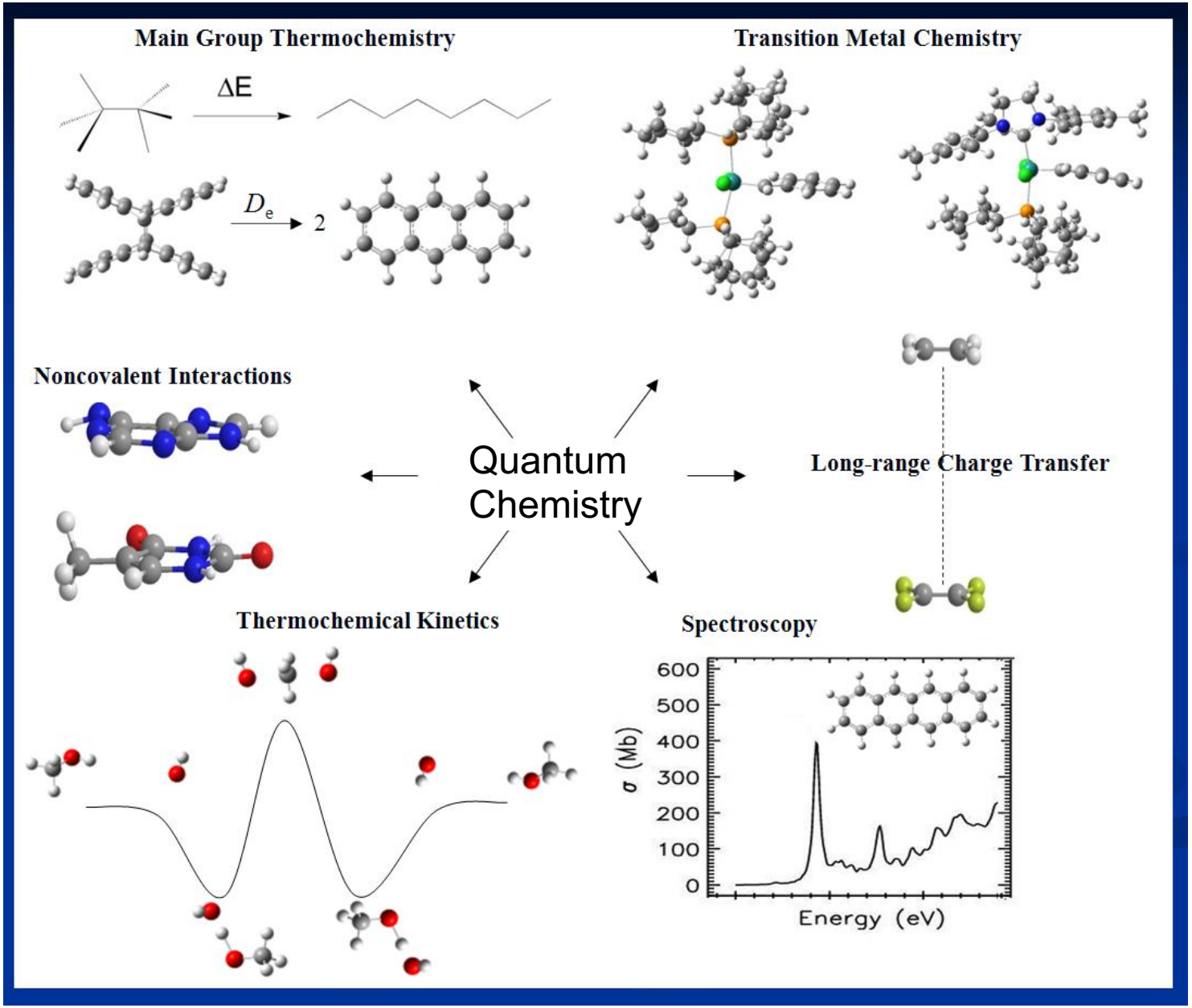
Conducting a Computational Project

- These questions should be answered
  - What do you want to know?
  - How accurate does the prediction need to be?
  - How much time can be devoted to the problem?
  - What approximations are being made?
- The answers to these questions will determine the type of calculation, model and basis set to be used ***Model Chemistry = Hamiltonian (method) + Basis Set***
- If good energy is the goal → use extrapolation procedures to achieve `chemical accuracy': G1/2/3, W1/2/3, PCI-80… models

* from D. Young

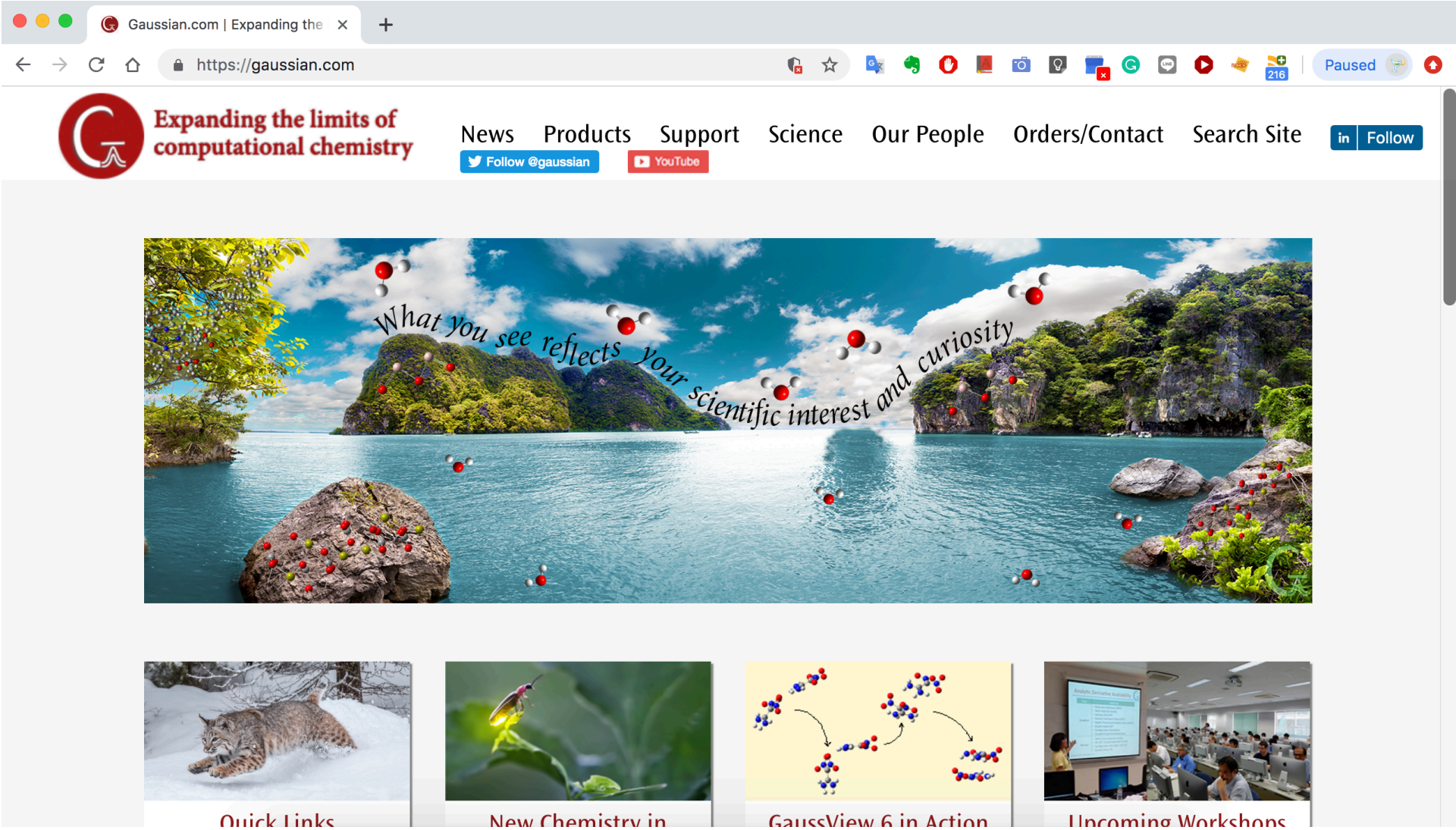
Variety of Methods in Computational Chemistry

	Quality	Size dependence
Ab initio MO Methods		
CCSD(T)	quantitative (1~2 kcal/mol) but expensive	~N^6
MP2	semi-quantitative and doable	~N^4
HF	qualitative	~N^{2-3}
Density Functional Theory		
DFT	semi-quantitative and cheap	~N^{2-3}
Semi-empirical MO Methods		
AM1, PM3, MNDO	semi-qualitative	~N^{2-3}
Molecular Mechanics Force Field		
MM3, Amber, Charmm	semi-qualitative (no bond-breaking)	~N^{1-2}



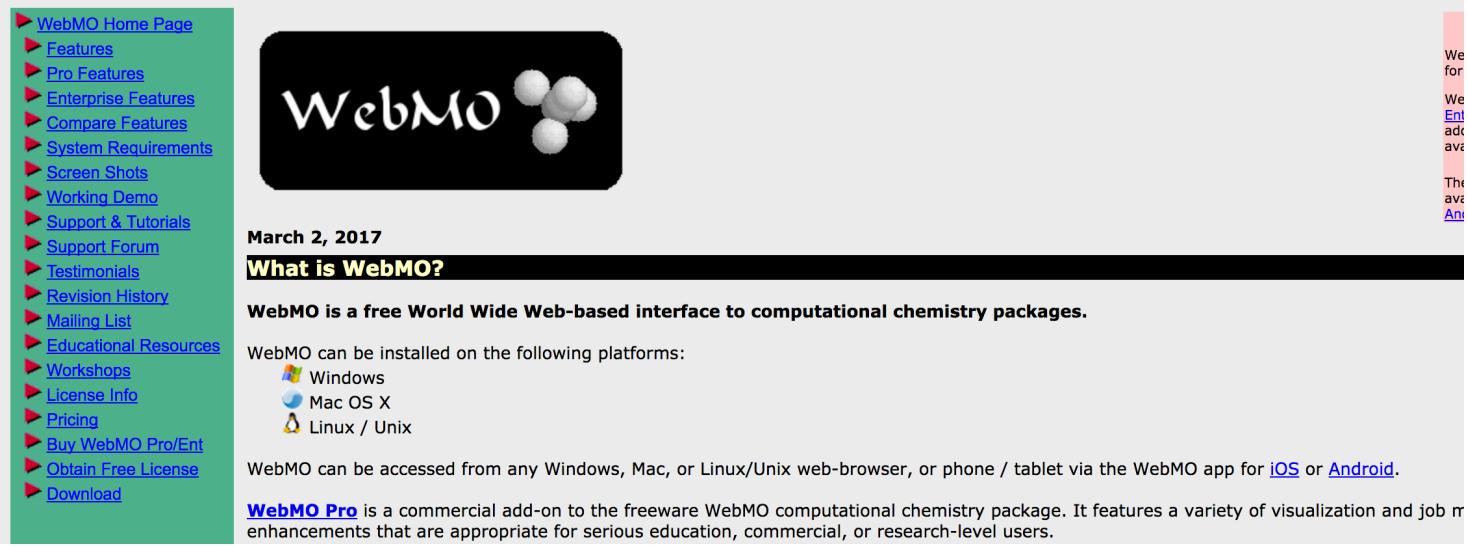
Courtesy of Donald G Truhlar

Gaussian Inc.



WebMO

- Computational Chemistry on the WWW: https://www.webmo.net/
- A simple GUI for various quantum chemistry calculations
- Supports for common quantum chemistry packages: Gaussian/Q-Chem/…



WebMO Server

- Computational Chemistry on the WWW: http://eos.ch.ntu.edu.tw/~webmo17/cgi-bin/webmo/login.cgi
- Login: username=guest, password = guest

WebMO Example: H_2^+

- Job manager: new job
- Build molecule: open editor, build H_2, clean up, next
- Choose engine: Gaussian
- Job options: MO, Hartree-Fock, basis, charge +1, meaning title, preview input file
- Submit job
- Job manager: view structure & MOs
- Electronic wave functions for H_2^+ (MOs)
- Examine Gaussian log file

WebMO Example: H_2CO

- Job manager: new job
- Build molecule: open editor, build H_2CO, next
- Choose engine: Gaussian
- Job options: Opt, B3LYP, basic basis, **preview input file**
- Submit job
- Examine Gaussian log file → steps taken in the calculation
- Job manager: view structure, properties
- Job viewer: new job using optimized geometry
- Submit MO job & repeat
- Job manager: view MOs, densities, electrostatic potentials

WebMO Example: H_2CO

- Job manager: H2CO Opt
- Job viewer: new job using optimized geometry
- Choose engine: Gaussian
- Job options: Freq, B3LYP, basic basis, **preview input file**
- Submit job
- Examine Gaussian log file → steps taken in the calculation
- Job manager: view structure, properties, **vibrations**

WebMO: What can be done?

- Single point calculation/MO analysis
- Geometry optimization → Opt
- Vibrational analysis/free energies → Freq
- Explore potential energy surface → Scan
- Excited states/solvation/… much more!!
- https://www.webmo.net/curriculum/index.html

WebMO Example: Builder

Examine various functions of the builder here:

- Job manager: new job
- HFCO: H_2CO → periodic table (O) → edit H to O → clean up (periodic table, edit molecules…)
- Ethene & benzene (double bond & clean up)
- $Pt(NH_3)_2Cl_2$ (periodic table, edit molecules…)
- cis-1,2-dicloroethene → trans-1,2-dicloroethene (adjust tool: bond, angle, dihedral angle…)
  Tools → Z-Matrix (detailed structure control)
- Build a benzene, check out Huckel orbitals
- more complicated molecules: c-hexane & molecules of your interest (Q & A)