

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

Variety of Methods in Computational Chemistry

Quality

Size dependence

■ ***Ab initio MO Methods***

- CCSD(T) quantitative (1~2 kcal/mol) but expensive $\sim N^6$
- MP2 semi-quantitative and doable $\sim N^4$
- HF qualitative $\sim N^{2-3}$

■ ***Density Functional Theory***

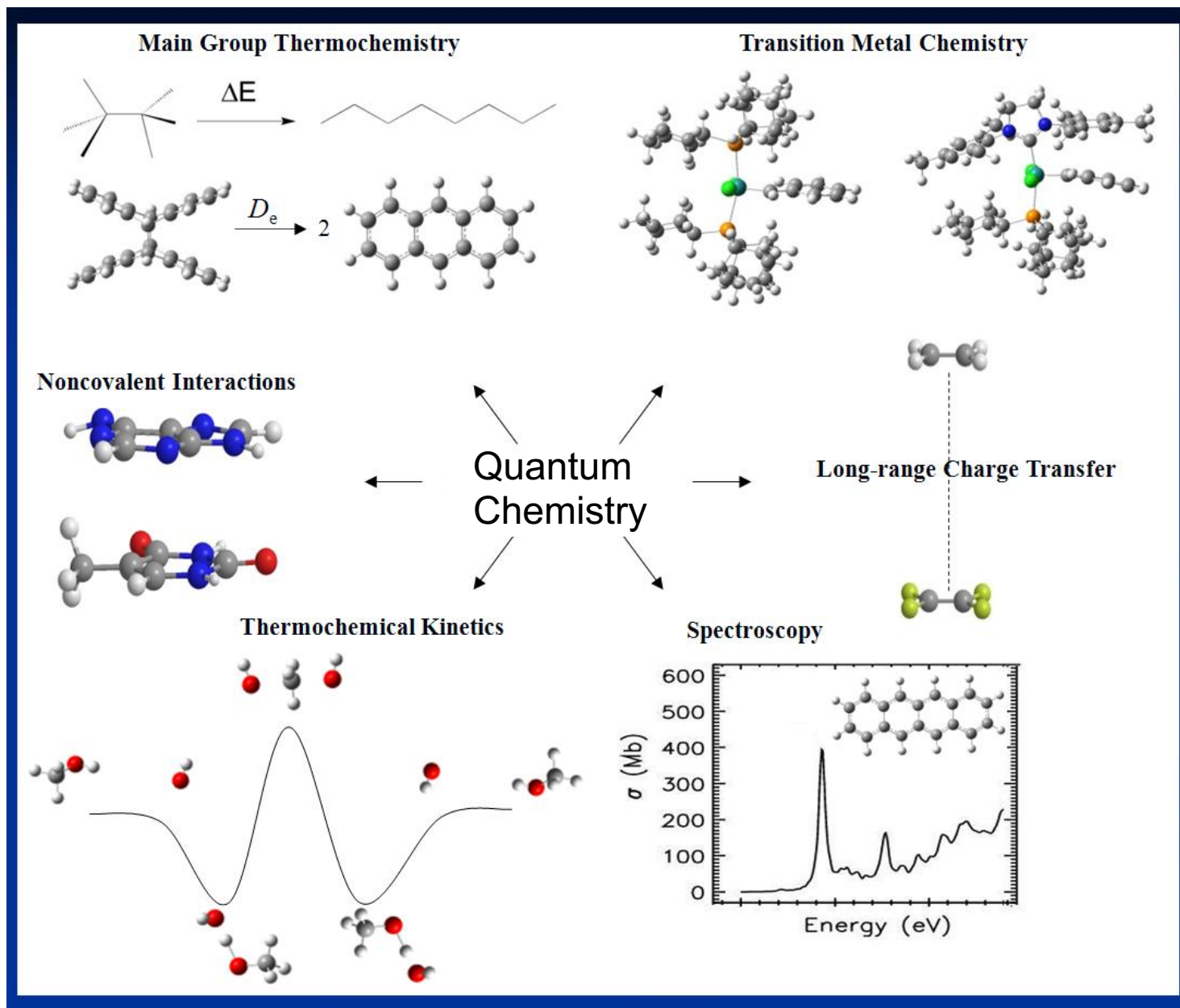
- DFT semi-quantitative and cheap $\sim N^{2-3}$

■ ***Semi-empirical MO Methods***

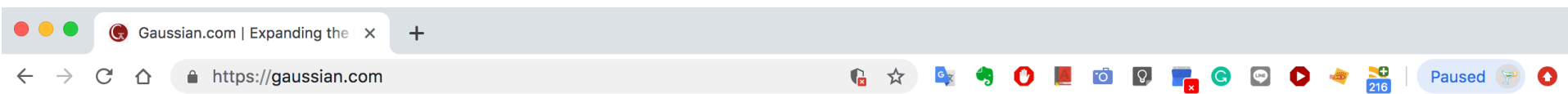
- AM1, PM3, MNDO semi-qualitative $\sim N^{2-3}$

■ **Molecular Mechanics Force Field**

- MM3, Amber, Charmm semi-qualitative (no bond-breaking) $\sim N^{1-2}$



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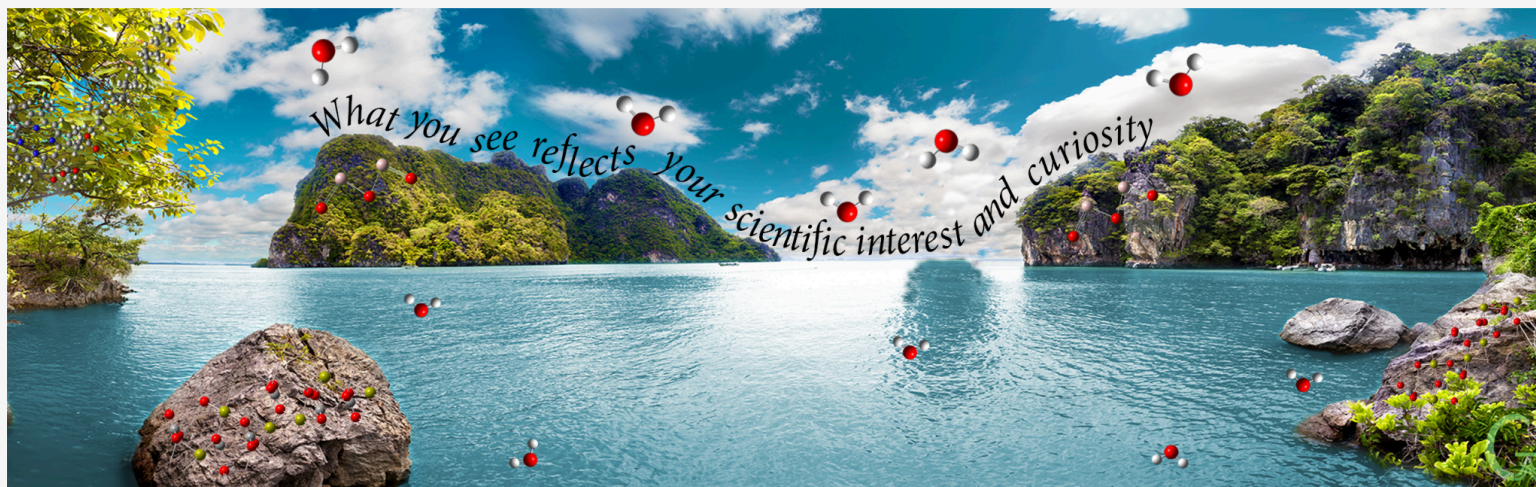
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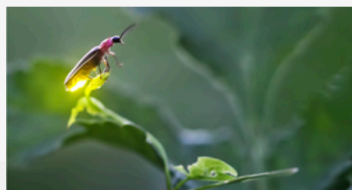
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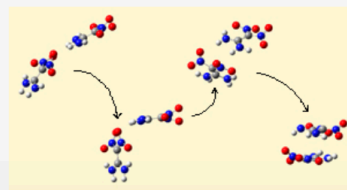
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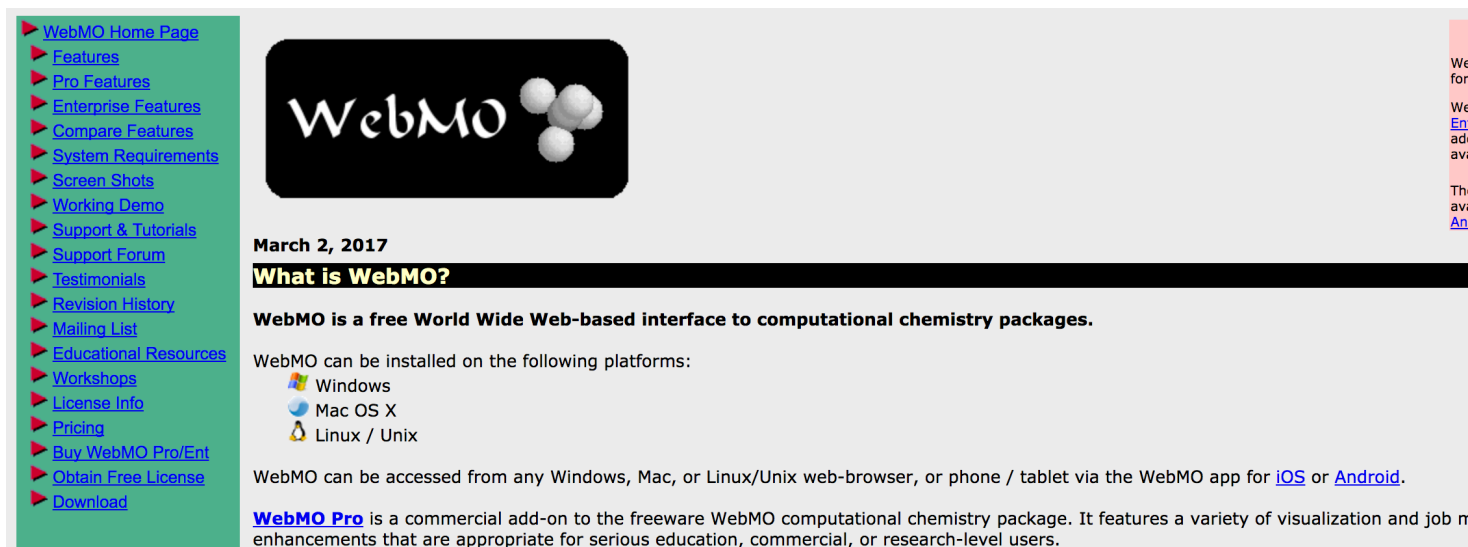
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WebMO

- 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/...



The screenshot shows the WebMO website homepage. On the left is a green sidebar with a list of links: WebMO Home Page, Features, Pro Features, Enterprise Features, Compare Features, System Requirements, Screen Shots, Working Demo, Support & Tutorials, Support Forum, Testimonials, Revision History, Mailing List, Educational Resources, Workshops, License Info, Pricing, Buy WebMO Pro/Ent, Obtain Free License, and Download. The main content area has a black header with the WebMO logo (the text 'WebMO' next to three white spheres). Below the header, the date 'March 2, 2017' is displayed. A black bar contains the text 'What is WebMO?'. The main text states: 'WebMO is a free World Wide Web-based interface to computational chemistry packages.' It then lists the platforms it can be installed on: Windows (with a Windows logo), Mac OS X (with an Apple logo), and Linux / Unix (with a Linux logo). Below this, it says 'WebMO can be accessed from any Windows, Mac, or Linux/Unix web-browser, or phone / tablet via the WebMO app for [iOS](#) or [Android](#).' At the bottom, it mentions 'WebMO Pro' as a commercial add-on to the freeware WebMO package, featuring visualization and job management enhancements for serious users.

WebMO Home Page
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WebMO

March 2, 2017

What is WebMO?

WebMO is a free World Wide Web-based interface to computational chemistry packages.

WebMO can be installed on the following platforms:

- Windows
- Mac OS X
- Linux / Unix

WebMO can be accessed from any Windows, Mac, or Linux/Unix web-browser, or phone / tablet via the WebMO app for [iOS](#) or [Android](#).

WebMO Pro is a commercial add-on to the freeware WebMO computational chemistry package. It features a variety of visualization and job management enhancements that are appropriate for serious education, commercial, or research-level users.



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: H₂⁺

- ☐ Job manager: new job
- ☐ Build molecule: open editor, build H₂, 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 H₂⁺ (MOs)
- ☐ Examine Gaussian log file

WebMO Example: H₂CO

- ☐ Job manager: new job
- ☐ Build molecule: open editor, build H₂CO, 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: H₂CO

- ☐ 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: $\text{H}_2\text{CO} \rightarrow$ periodic table (O) \rightarrow edit H to O \rightarrow clean up (periodic table, edit molecules...)
 - ☐ Ethene & benzene (double bond & clean up)
 - ☐ $\text{Pt}(\text{NH}_3)_2\text{Cl}_2$ (periodic table, edit molecules...)
 - ☐ cis-1,2-dichloroethene \rightarrow trans-1,2-dichloroethene (adjust tool: bond, angle, dihedral angle...)
- Tools \rightarrow Z-Matrix (detailed structure control)
- ☐ Build a benzene, check out Huckel orbitals
 - ☐ more complicated molecules: c-hexane & molecules of your interest (Q & A)