Computational Chemistry in Community College Education and Research: Learning about Periodic Trends and Materials Design from First-Principles Calculations

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HAWKEYE COMMUNITY COLLEGE

THE UNIVERSITY OF IOWA

Hawkeye Community College's Mission

Mission: A globally informed community of successful lifelong learners

To do this, show students how modern science is done, regardless of their goal degree.

Need to build bridges between the community, Hawkeye and the 4-year institutions in Iowa

- Outreach
- Education
- Research

www.hawkeyecollege.edu/stem

How does Computational Chemistry Fit the Mission?

- Data science is a growing field; opportunity to incorporate coding into chemistry.
- Students who participate in research are better prepared for both transfer and workplace opportunities.
- Guided Inquiry is emerging as a better means for comprehensive chemical education and concept retention.
- Computational chemistry incorporates all of these!

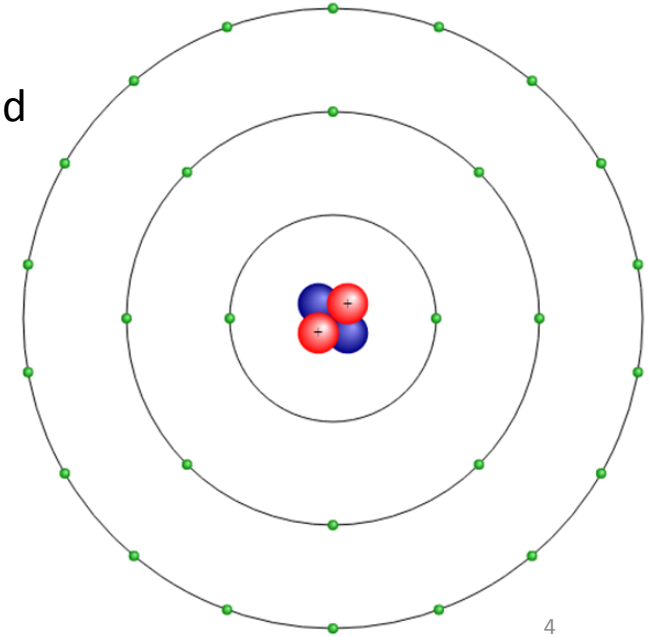
Tapping the Potential of All: Undergraduate Research at Community Colleges, 2014

Computational Chemistry and First-Year Courses

Computational chemistry not typically introduced early in student careers.

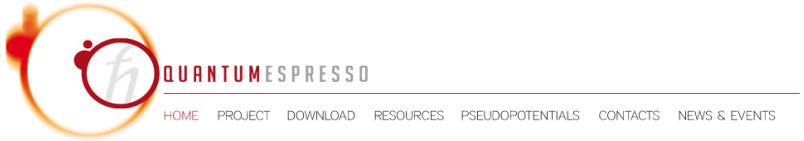
- The few exceptions:
  - Molecular modeling using PC Spartan Pro or Gaussian (Feller *et al*, Pearson)
  - Quantum Mechanics for Honors Students (deSouza and Iyengar)

- Useful tool for teaching electronic structure!
  - What's needed?
    - Knowledge
    - Computers
    - Software…$$$?



S. E. Feller, *et al*., *J. Chem. Educ.,* **81***,* 2 (2004).
J.K. Pearson, *J. Chem. Educ*., **84**, 8 (2007).
R.T. deSouza, *J. Chem Educ*., **90**, 6 (2013).

Open-Source Codes



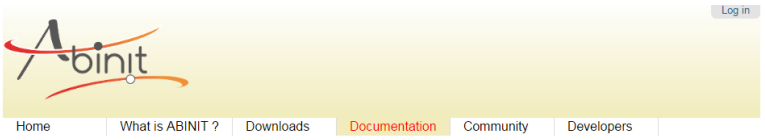
Pros

- Free
- Can install on numerous computers
- Tutorials available
- User Forums
- Codes can be edited as desired

Cons

- Not as User Friendly as Commercial
- Tech Support Relies on Forums
- Steep Learning Curves
- Tutorials not designed for classrooms

Open-Source Pseudopotential Interface/Unification Module (OPIUM)



http://www.allwhitebackground.com/computer-white-background-images

My Computational Chemistry Exercises at Hawkeye

Structured

- Questions and procedures provided
- Elements and ions assigned to students
- Directions on data organization and necessary graphs provided
- Data analysis questions. Do students "understand material"?

Guided Inquiry

- Preliminary Activity
- Questions provided
- Students develop plan to obtain necessary data
- Data interpretation used to determine correct configuration
- Students determine how to best present data to answer questions

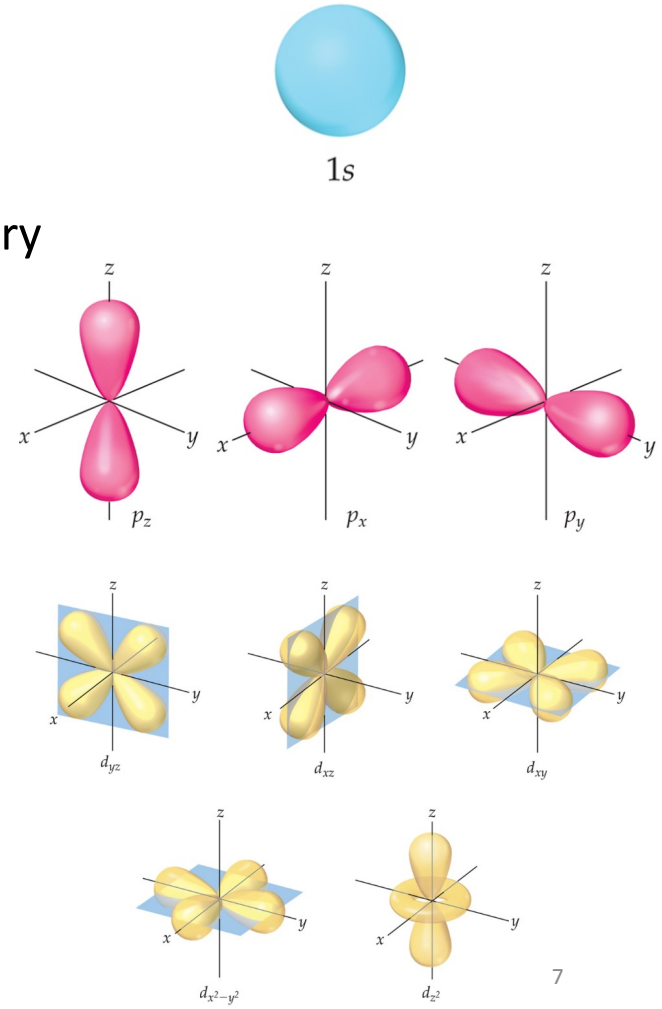
Quantum Chemistry and Spectroscopy: A Guided Inquiry: Tricia D. Shepherd, Alexander Grushow, 2014

Electronic Structure of Atoms

- Chapter 6: Brown and Lemay
- Concepts to teach through computational chemistry
  - Quantized energy
  - Electron configurations
  - Many-electron atoms
  - Periodic trends

- Example: My Exploring the Aufbau Principle Computational Lab
  - 2 years running
  - 250 students total.

OPIUM: All-electronic quantum mechanics of atom calculations.



Building an Atom

- 3 required keyblocks for the input file

[Atom]

C

3

100 2.00 - 1s

200 2.00 - 2s

210 2.00 - 2p

[Pseudo]
2 1.4 1.4
opt

[Optinfo]
7.07 10
7.07 10

- What atom is being examined
- How many sublevels does the atom contain
- Quantum numbers (Column 1)
  - n is the energy level
  - l is orbital angular momentum and is equal to n-1 (s, p, d, f)
  - m is the magnetic component , 0 for OPIUM
- Occupation = number of electrons in orbital (Column 2)
  - s can hold up to 2
  - p can hold 6
  - d can contain 10
  - f can have 14
- Last column is for energy guesses.
  - OPIUM guesses for -

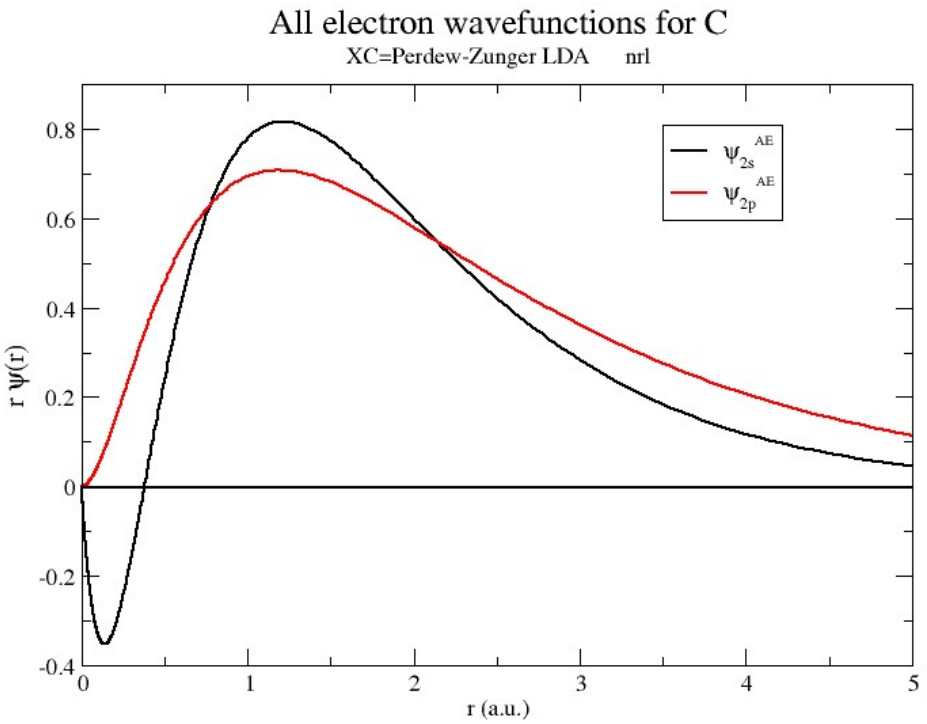
[Pseudo]
No. of valence orbitals
Radius of valence orbitals

[Optinfo]
Cutoff wavevector
No. Bessel functions

Running Calculations

- Command to run calculation:
  ./opium C C.log ae rpt plot wa

- ae -- Runs all-electron calculations
- rpt – Creates report file and stores results
- plot wa –plots all-electron wavefunction



Extracting Data: All-electron Report

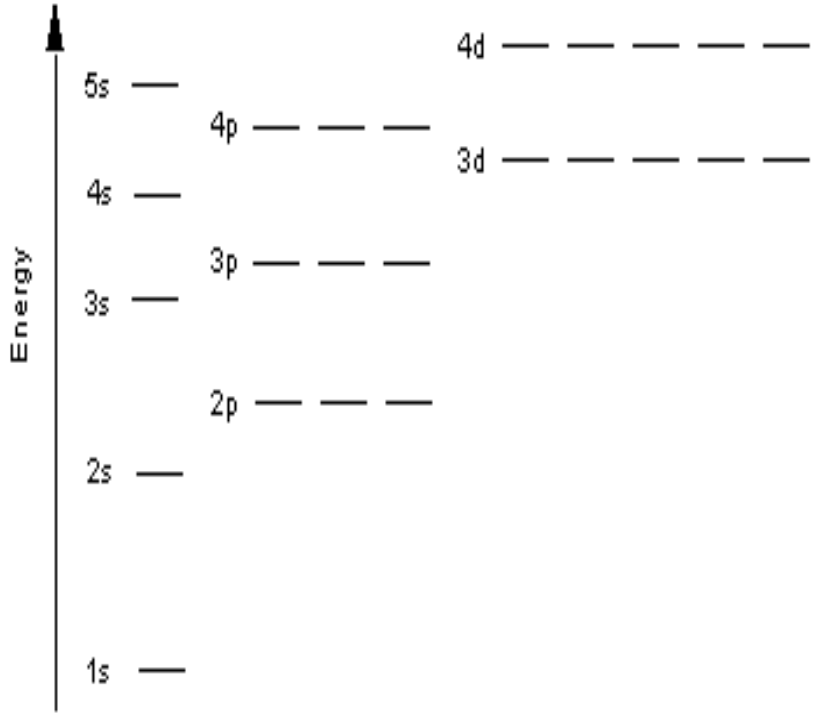
AE report

AE:Orbital	Filling	Eigenvalues[Ry]
100	2.000	-19.895705
200	2.000	-1.001950
210	2.000	-0.398599

E_tot = -74.84852399 Ry

- Eigenvalues are the orbital energy in Rydberg
- Which occupied orbital has the lowest energy?
- Which one has the highest?
- Sketch out an orbital filling diagram based off of the energies.
  - Does this match the text diagram?
- What is the total energy?
- Repeat with elements, ions or other configurations

Lab Questions:



- How can the correct electron configuration be identified?
- Is the Aufbau Principle obeyed in all instances?

Configuration Comparison: Fe

AE:Orbital	Filling	Eigenvalues[Ry]
100	2.000	-509.5784725199
200	2.000	-59.2595645575
210	6.000	-51.1378442569
300	2.000	-6.7576140984
310	6.000	-4.3828175418
400	2.000	-0.3822532208
410	0.000	-0.0993588416
320	6.000	-0.5715390813

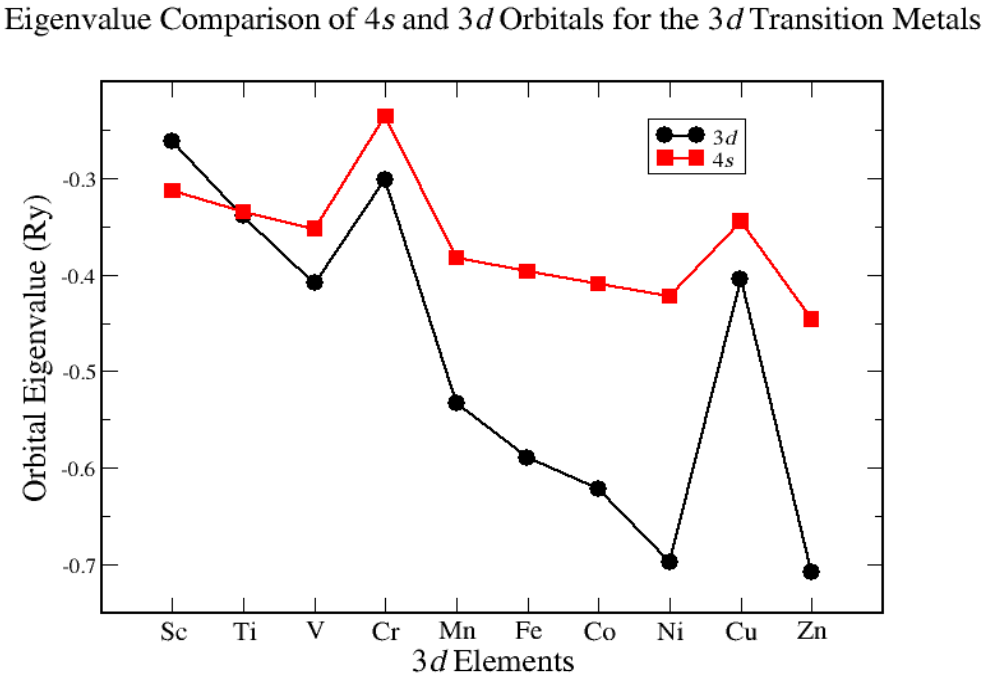
E_tot = -2526.5917748755 Ry

AE:Orbital	Filling	Eigenvalues[Ry]
100	2.000	-509.0380549307
200	2.000	-58.6488544800
210	6.000	-50.5342850513
300	2.000	-6.2806235923
310	6.000	-3.8410033951
400	2.000	-0.2547850662
410	0.000	-0.0461290565
320	8.000	-1.7353081083

E_tot = -2526.5907444971 Ry

Is Aufbau Obeyed?

- Students contribute to class database
- Create graphs for their elements
- Use this database to examine Aufbau Principle
- Identify instances in which Aufbau is not obeyed
- Determine which orbitals will lose electrons



Student Feedback from Exercises

Things that went well

- Enhanced comprehension of subshell filling
- Greater understanding in why 4*s* e^- are removed before 3*d* e^-
- Testing of cation configurations
- Excitement over computational exercise

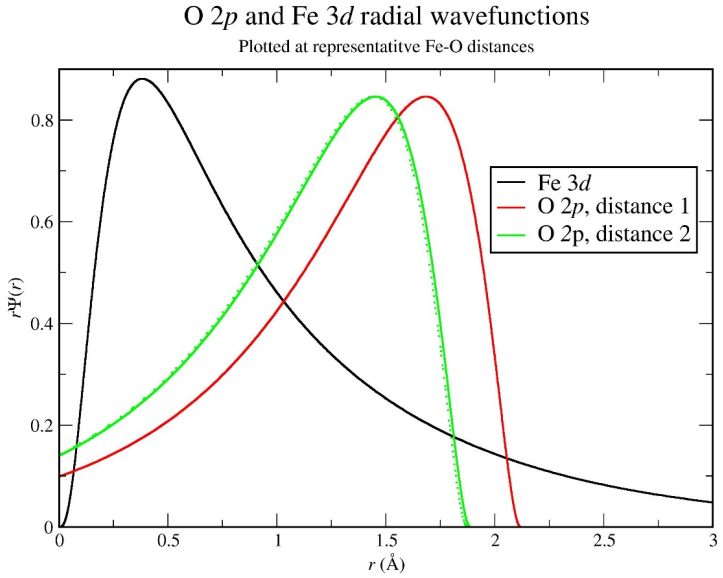
Things that didn't go well

- Spelling/Typing errors
  - Results in technical issues
- Naming files
- Forgotten spaces
- Significant digits
- Anions—known code issue

Going Beyond Aufbau

- Periodic trends
- Ionization Energy Calculations
- Unit Conversions
- Molecular Orbital Prediction
- Hybridization

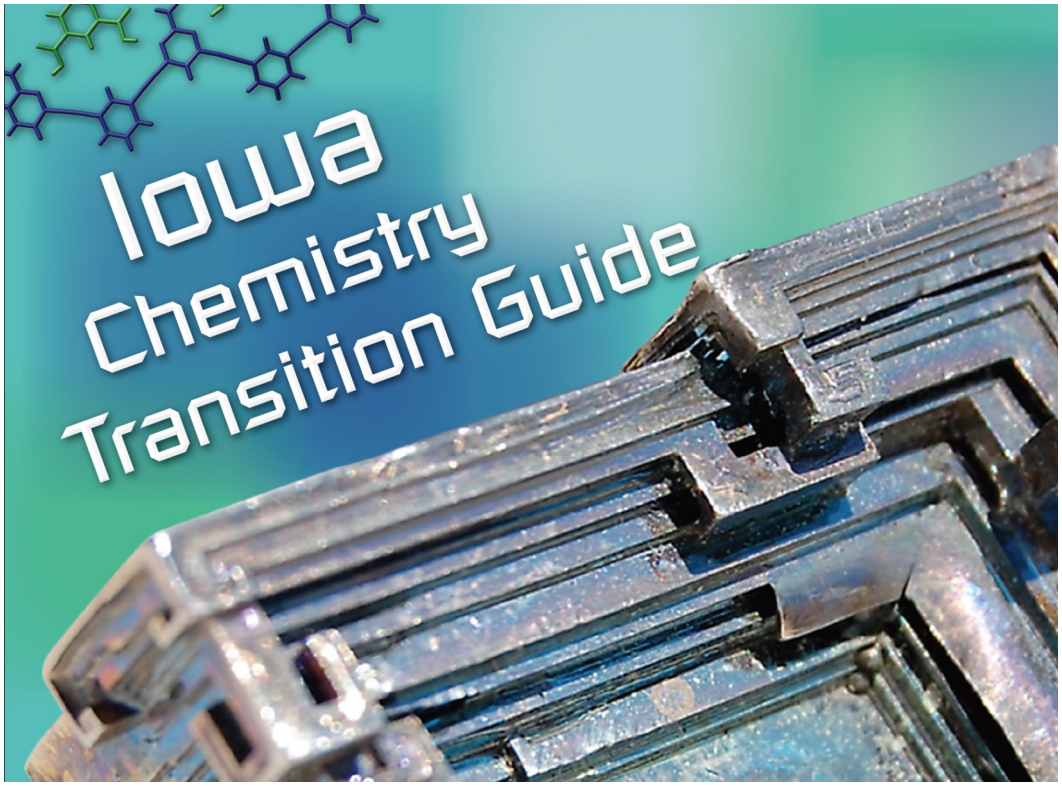
- Not just for first-year students!
- Applications in Physical Chemistry courses
- Graduate Quantum Chemistry



Greater understanding on applications of computational chemistry!

Transferable Skills

- Exercise not only introduces students to computational chemistry, but helps develop skills necessary for a successful transfer
  - Computer skills
  - Quantitative Reasoning
  - Critical Thinking
  - Communication



http://www.transferiniowa.org/transition.php

Building Bridges: Hawkeye Community College and the University of Iowa

- Dr. Sara E. Mason visits after these lab exercises
- Discuss computational chemistry research at the University of Iowa and how it pertains to an array of fields
  - Agriculture
  - Environmental Science
  - Materials
  - Medicine
- Research opportunities for undergraduates at Hawkeye Community College and The University of Iowa

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CAREER

Questions?

QCC For Everyone