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Water in the Computer Lab! (A Computational Project for Undergraduate Inorganic Chemistry)

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A computational project for undergraduate inorganic chemistry students

Bradley M. Wile and Trilisa M. Perrine

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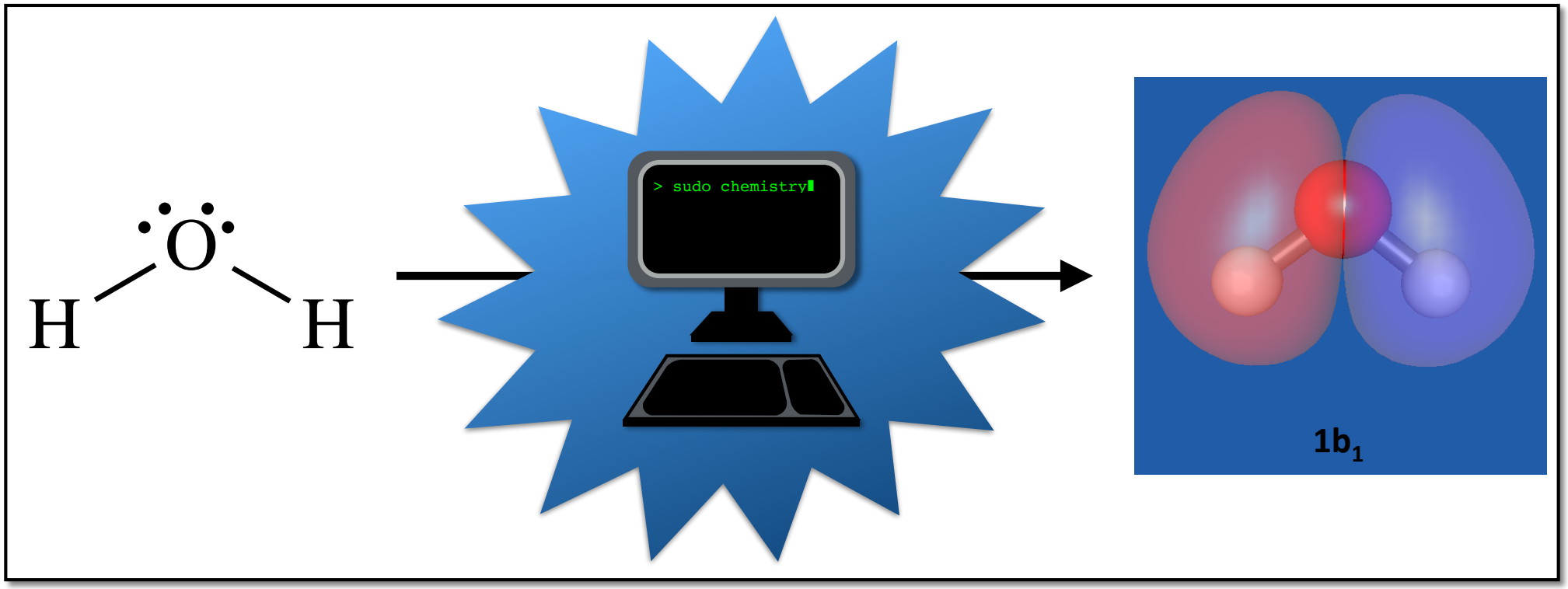
OHIO NORTHERN UNIVERSITY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Today's talk

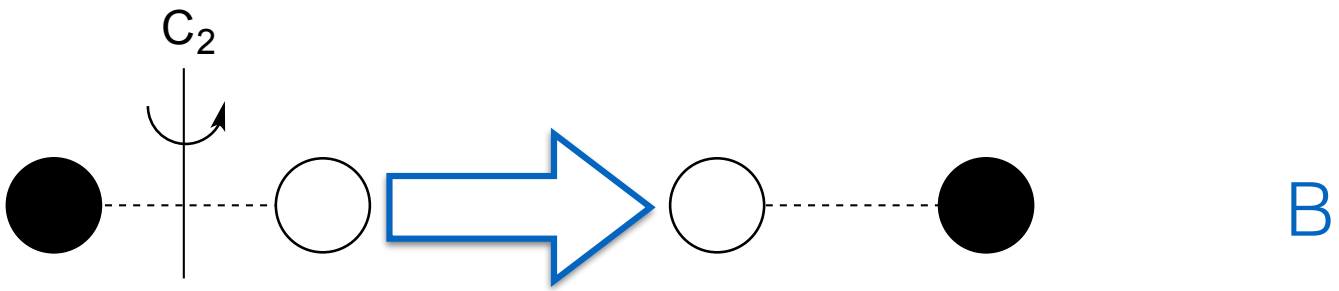
- Course structure/background
- Motivation for the project
- Methods used
- Student results
- Issues and future directions

Inorganic Chemistry 2

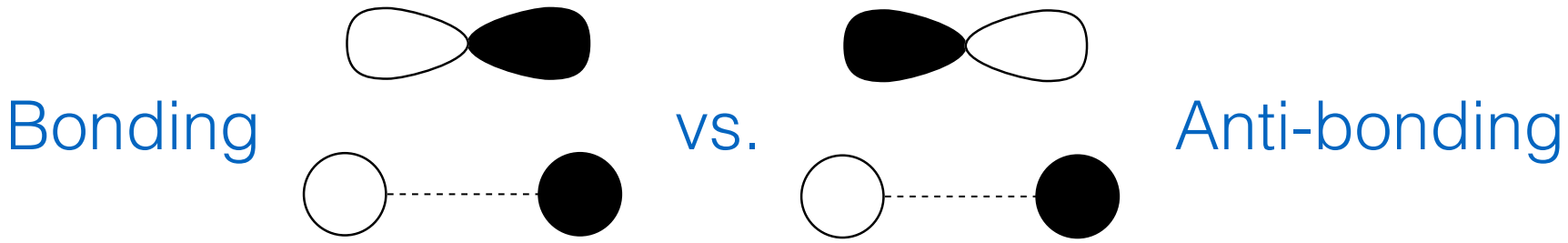
- Chem 4721 - “Advanced inorganic”
  - Junior or senior students
  - Entirely elective
- Spring semester, every second year
  - Same schedule/semester as computational class (Advanced Topics in Physical Chemistry)

Course Background

- Have covered point groups/symmetry
- Determining symmetry of H···H LGOs (e.g. A vs. B)



- Combination of symmetry matched orbitals



Course Material & Timing

Atomic structure, shielding, & orbitals	Molecular symmetry Vibrational modes, LGOs/SALCs	Combining LGOs & AOs to form an MO diagram	Review diatomic MOs, on to NH_3 & CH_4, correlation diagrams	…

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…

Probably makes more sense to run activity here…

Goals

- Reinforce matching of orbitals (AOs/LGOs) by symmetry
  - See the shape of MOs vs. qualitative sketches
- Get a feel for the scale (ΔE) for a simple system
- Understand the differences between a quantitative and a qualitative MO diagram

Assignment

Project 1 - Water

In this assignment, you will use computational software to visualize the MOs for a simple inorganic compound, water. Ultimately, you will prepare an MO diagram, depicting the energy of the corresponding O AOs and H···H LGOs and the H_2O MOs, as well as the shape of each MO. You will work in groups of two for this exercise.

Day 1 - Set up and execute the calculations at an appropriate level of theory.

Day 2 - Visualize the MOs, and determine the symmetry and energy for each.

Day 3 - Construct your diagram for water with scaled spacing between orbitals.

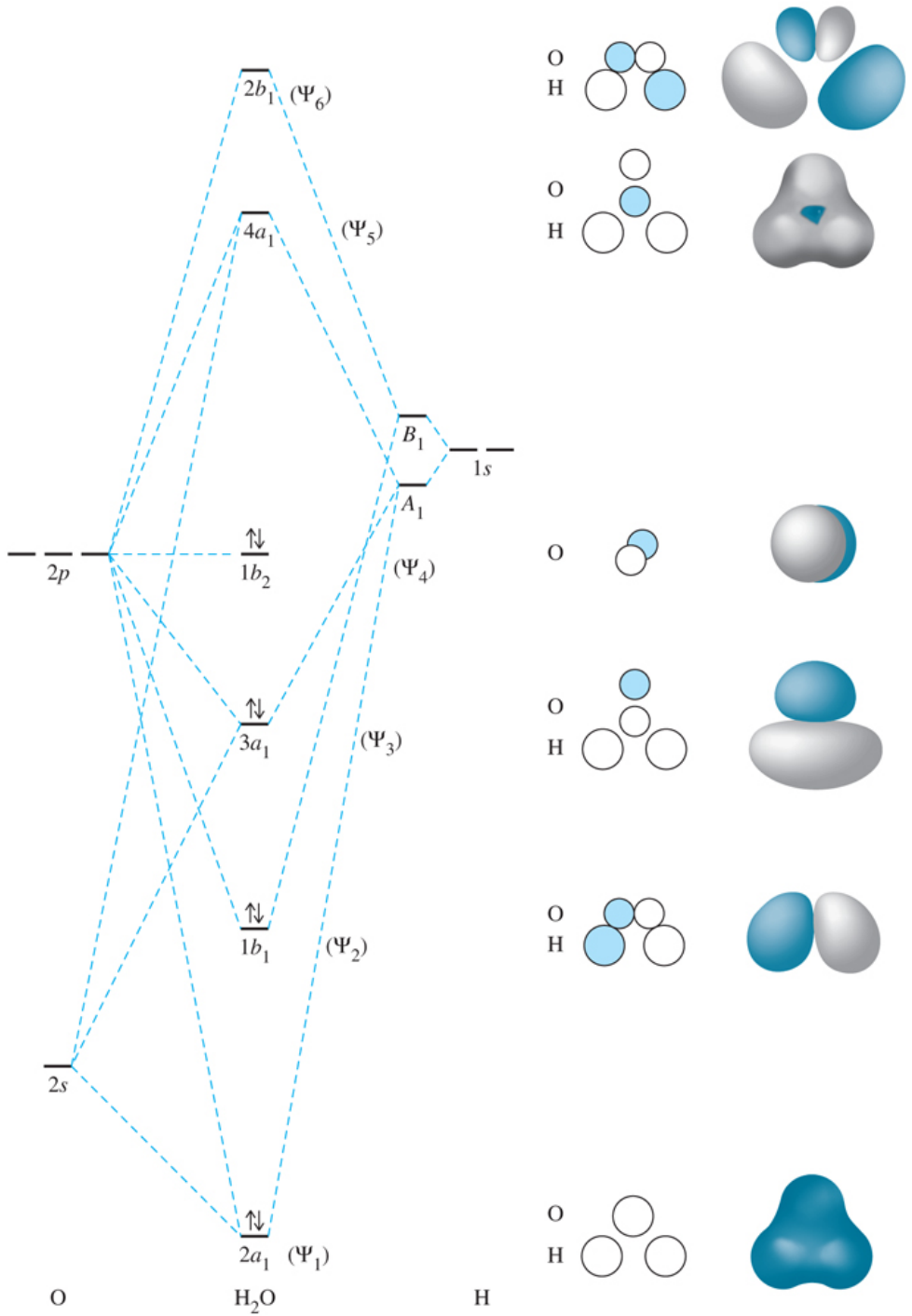
Submit your completed MO diagram to the course Moodle page. We will discuss the preparation of qualitative MO diagrams using an LGO approach in class, so you may wish to bring a copy of your diagram with you.

Methods

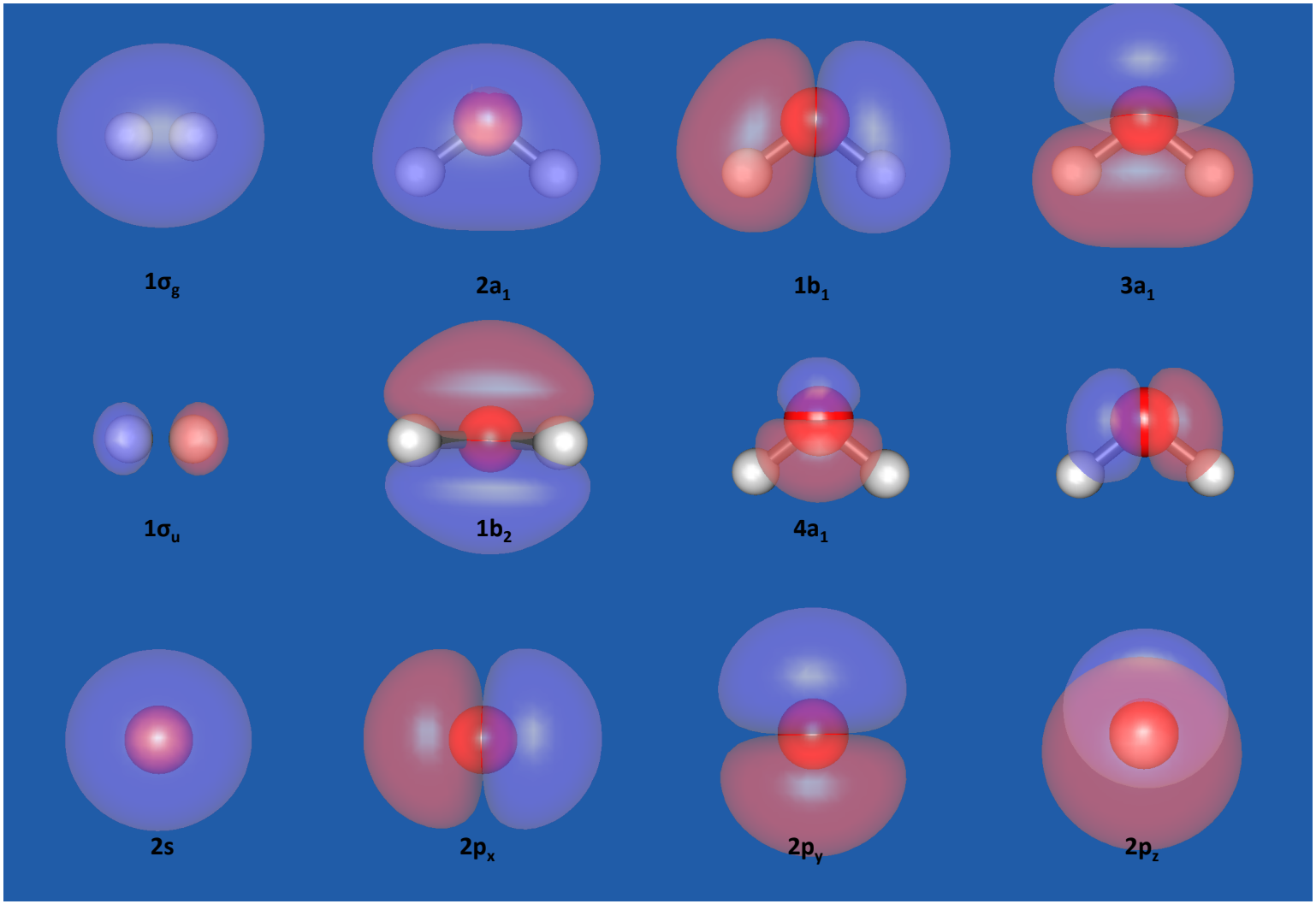
- Build and visualize using IQmol
- Calculations run using Q-Chem
- MP2 with 6-311++G**
  - One student tried basis sets STO-3G/6G, 6-31G*, and cc-pCVDZ
- Energies of H_2 instead of H···H LGOs

Ideally…

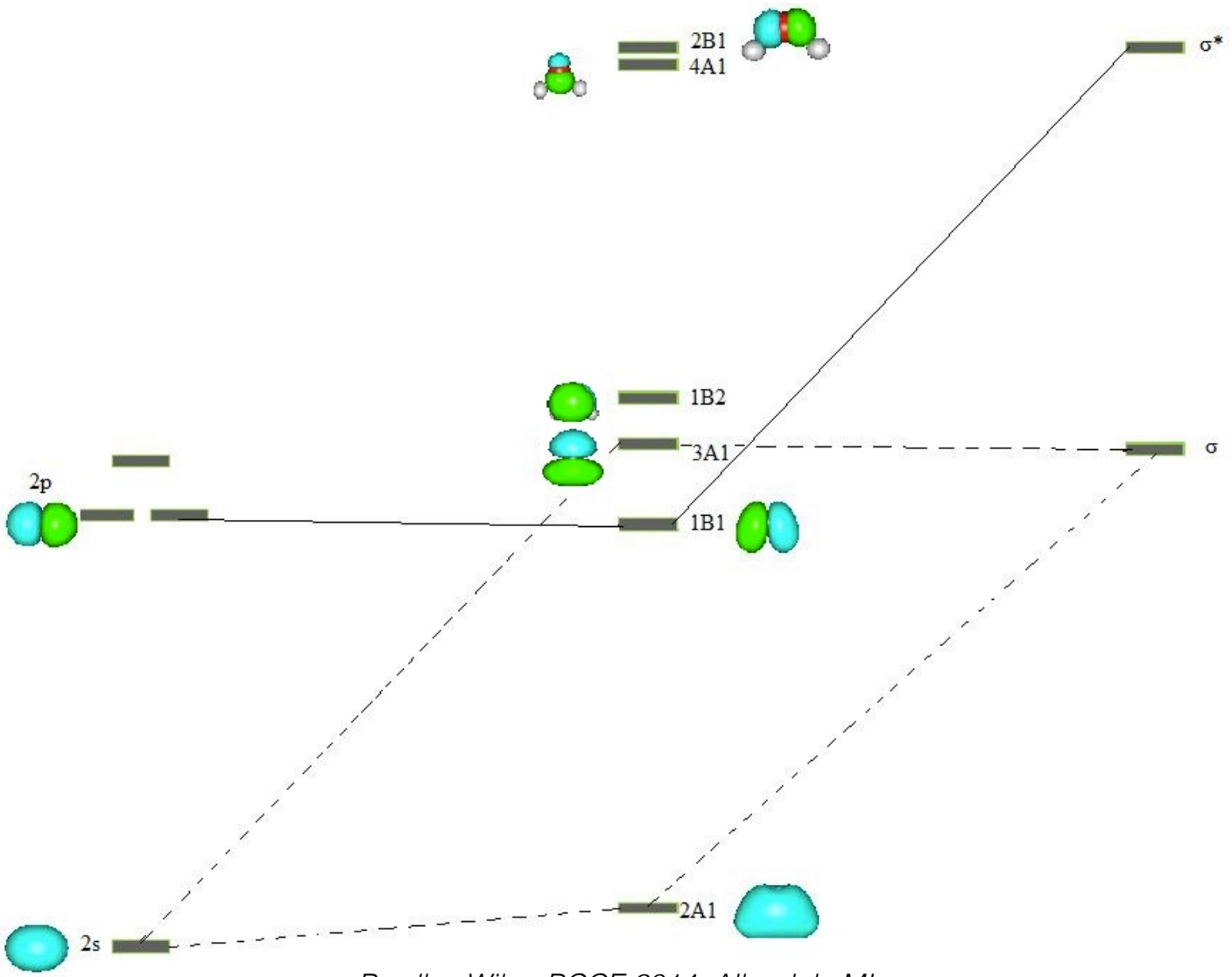
- "back of the envelope" idealized MO diagram
  - Qualitative…



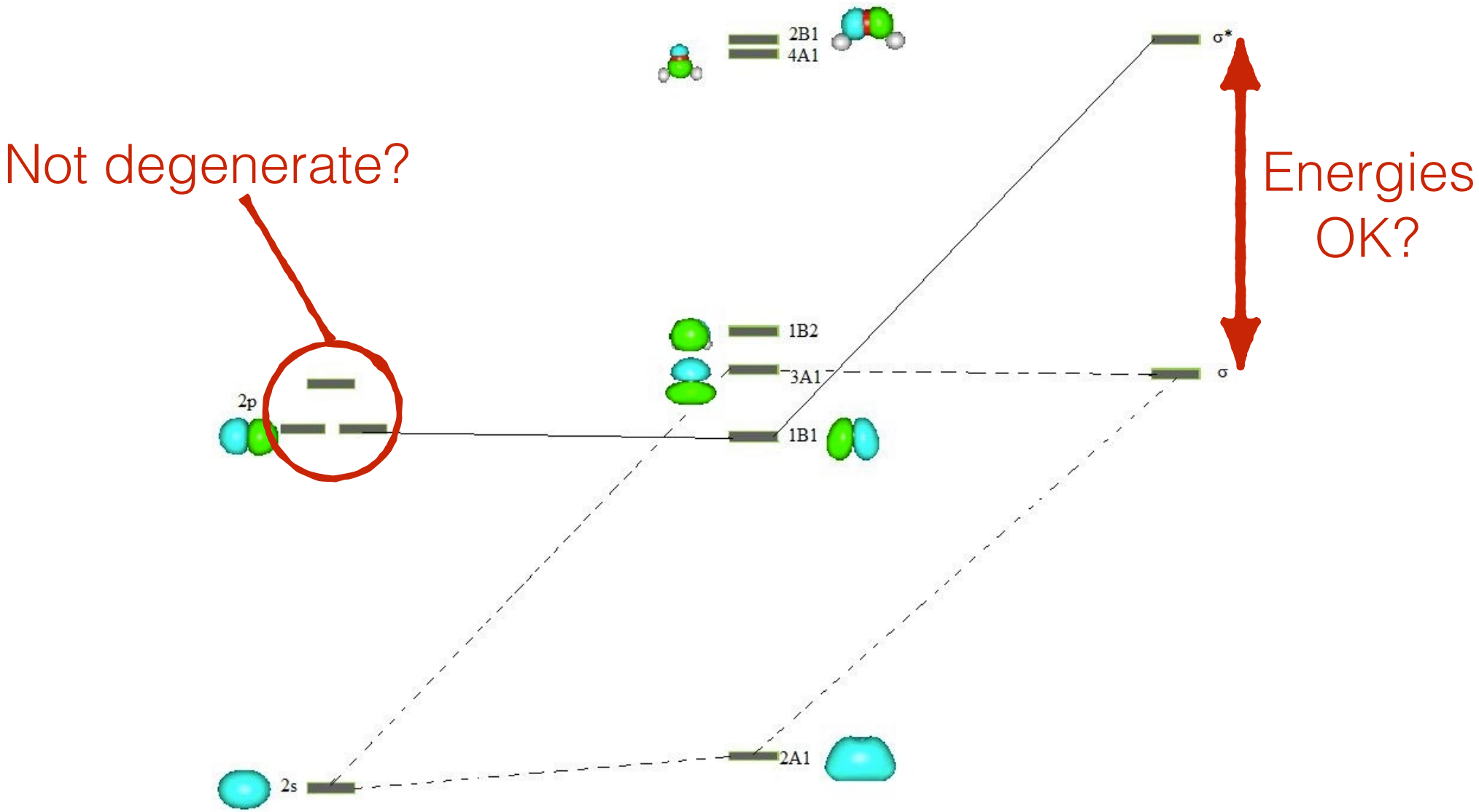
Student output (atypical)



Student output (typical)

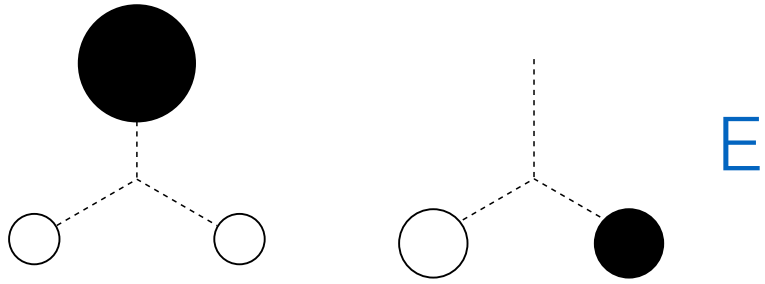


Issues…

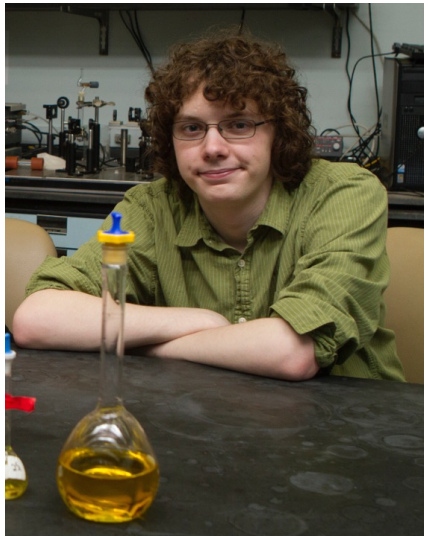


Future Directions

- More robust discussion of LGOs prior to exercise
  - Calculate using H···H LGOs
- Alternatives to H_2O (avoid problems with O atom)
  - NH_3 - N atom has a quartet GS 😀
  - LGOs less obvious 😟
- More pointed questions!



Acknowledgements



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- You - for staying, listening, and suggestions/questions!