Atomic energy levels and line spectra

In this activity, you will use an animation and various simulations to learn how photoelectron spectroscopy works and how spectroscopic techniques can help us draw conclusions about electron configurations, energy levels, and orbitals in atoms.

Link to the simulations for this activity: https://tcel-hu-berlin.github.io/silc/index_EN.html

= hint available on the website = discussion point BONUS = low-priority question

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Preparation Exercises

1. Before starting the activity, take a moment to familiarize yourself with the terms *shell*, *subshell*, and *orbital*. To check your understanding, match each of the three terms to its corresponding quantum number and to an example.

Term	**Quantum Number**	**Example**
shell	l	2p
subshell	n	$2p_x$
orbital	m_l	L

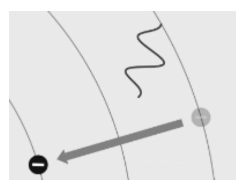
2. View Animation A and its accompanying description to learn more about the principles of photoelectron spectroscopy (PES). Then, switch to Simulation A and answer the following question:

   The ionization energy needed to remove an electron from each subshell increases from right to left along the x-axis. Which of the following statements is correct?

   I. The subshells on the left side of the x-axis lie at a <u>lower</u> energy level than the subshells on the right side of the x-axis.

   II. The subshells on the left side of the x-axis lie at a <u>higher</u> energy level than the subshells on the right side of the x-axis.

3. Open Simulation B. Play around with adjusting the initial and final positions of the transition arrow. Occasionally, you will see a squiggle like the one on the right appear. What does it represent and under what conditions does it appear?



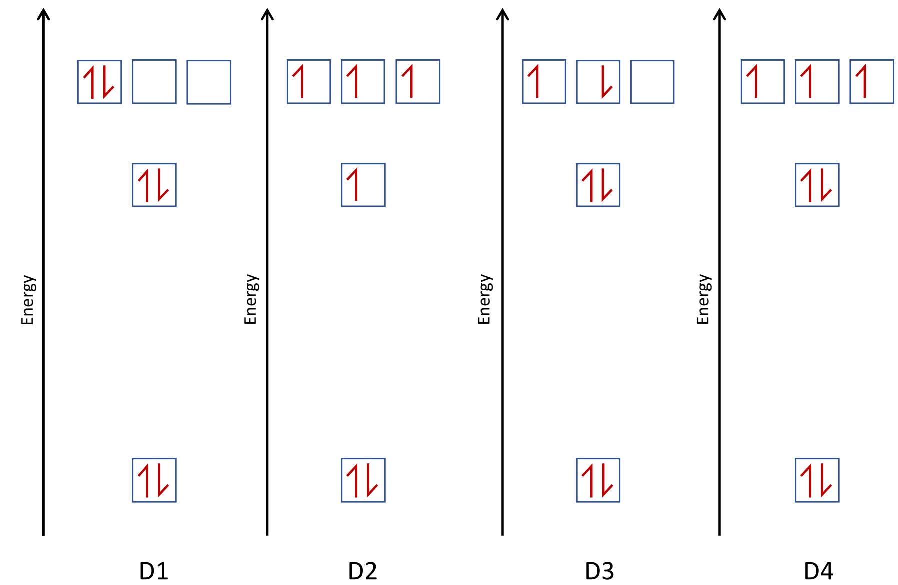
Main Exercises

1. Display the spectrum for element U1 and make a rough sketch of it below. Assuming all the subshells of the element are represented in the spectrum, label the peaks of the PES spectrum according to which subshell they correspond to (1s, 2s etc.).

2. Using information from the graph about how many electrons are present in each subshell, write out the ground-state electron configuration of element U1. For reference, the ground-state electron configuration of Lithium is $1s^2 2s^1$.

3. Determine the identity of U1, assuming it is a neutral atom.

4. Below are some suggestions for the atomic orbital diagram of element U1 in its ground state.



Discuss each of the diagrams D1-D4 with your peers and state:

a) if it is consistent with the PES spectrum and why/why not.

b) Which rules about building ground-state electronic configurations are violated, if any.

5. Provide the correct atomic orbital diagram of element U1. Note that the correct answer may not be included in the options D1-D4.

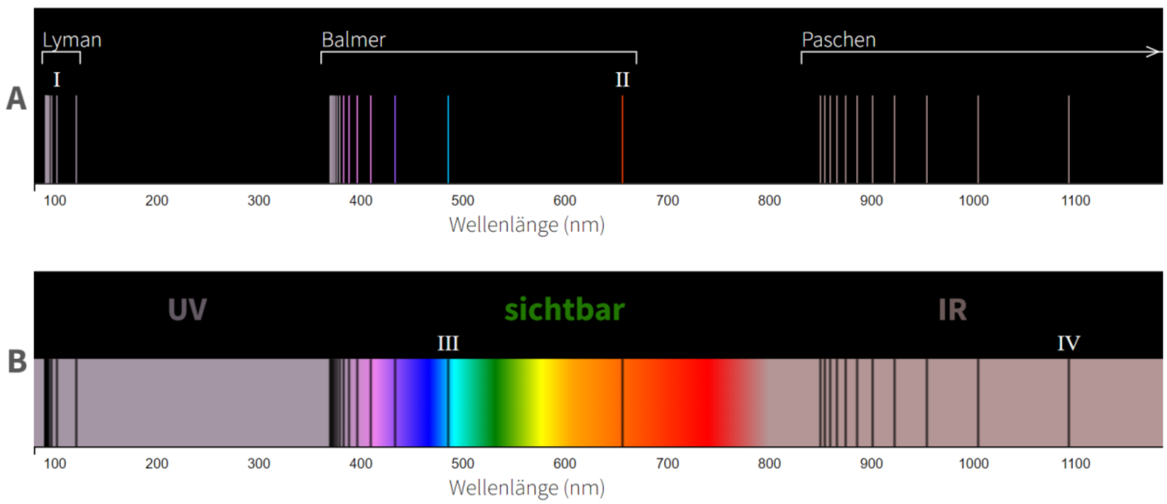
BONUS 6. Write out the electron configuration, state the identity of, and sketch the atomic orbital diagrams for the unknowns U2-U5. Ensure that all electron configurations are consistent with the PES spectrum! You can assume that all unknowns are neutral atoms and that all of their subshells are represented in their PES spectra. Check your answer with your peers.

7. You may have noticed that the electron configuration of U4 seemingly violates the normal ordering rule of electrons in energy levels. Explain how the rule appears to be violated and why the electron configuration is nevertheless correct.

Open Simulation B und read through the overview

8. The energy is represented both as wavelength (in nm) and as electron volts (eV) in the simulation. Which mathematical expression can you use to convert nm to eV? Check your answer with one of the available pairs of (nm, eV) values in Simulation B.

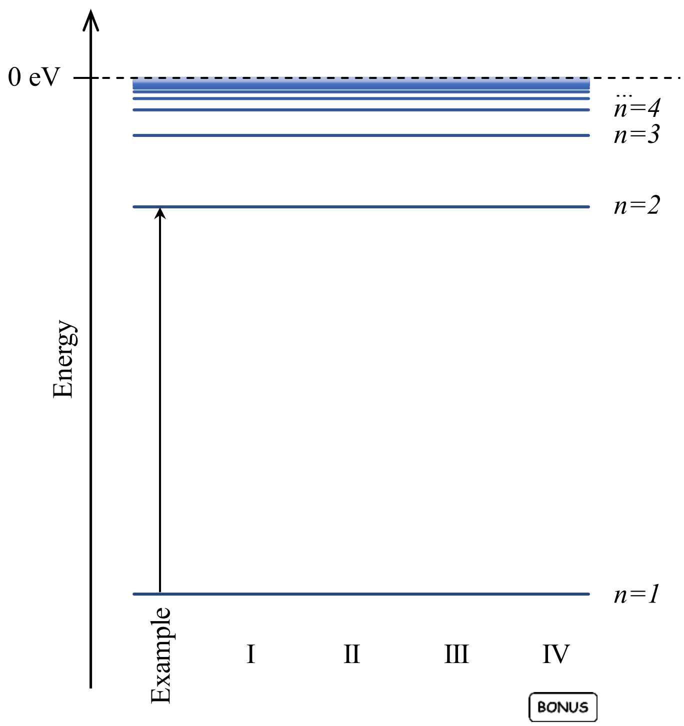
9. Take a look at the line spectra A and B and answer the following questions. An interactive version of the spectra can be found in the Help menu.



a) Out of the two spectra, which one is an <u>absorption</u> spectrum, and which one is an <u>emission</u> spectrum? Justify your answer.

b) In spectrum A, groups of lines are labeled Lyman, Balmer, and Paschen. This distinction has to do with the type of energy transition that results in each line. What do all the lines in the Lyman series have in common? What about the lines in the Balmer and Paschen series?

c) Draw arrows on the energy diagram below to represent the energy transitions that are responsible for lines I-III (as BONUS: also IV).



10. The next goal is to determine the relationship between the quantum number *n* and the energy that corresponds to it.

a) The lowest energy level (quantum number n=1) in the hydrogen atom lies at -13.6 eV. Use Simulation B to determine the energies, in eV, of energy levels with quantum number *n* = 2-8.

n	*E* (eV)
1	-13.6
2	
3	
4	
5	
6	
7	
8	

b) Enter the energies you calculated into the table of Interactive Graph B. When you are finished, you should see them plotted on the screen.

c) Go to the "Algebra" tab of Interactive Graph B. On the left, you should see an equation of the form $E(x) = a\, x^b$, where you can adjust the parameters *a* and *b*. Determine the set of parameters *a* and *b* that best agree with your "measured" values of energy.

a: _______ *b:* ________

d) Based on your answer to c, what mathematical equation describes the energy E(*n*) of an energy level with quantum number *n*, according to the Bohr model?

e) Given your answer to (d), what general mathematical form can be used to determine the energy *difference* (ΔE) for a transition between two energy levels? Let the quantum numbers of the energy levels be $n_{initial}$ and n_{final}.

f) Using the formula you derived, calculate the energy in eV of the following transitions and classify them as absorptive or emissive. In addition, calculate the wavelength in nm and the frequency in Hz for each transition. Finally, state what region of the electromagnetic spectrum (e.g. UV, visible, or IR), the energy corresponds to.

	$n_{initial}$	n_{final}	Absorption or emission?	Transition energy (eV)	Transition wavelength (nm)	Frequency (Hz)	Spectral region
	2	5					
	4	3					
BONUS	6	1					

Open Simulation C und read through the overview.

11. Try visualizing the orbitals for various combinations of the quantum numbers n, l and m_l in the simulation. Discuss which property of an orbital (e.g. size, direction, shape) is best represented by each quantum number. Summarize your thoughts in the following table and state the formal name of each quantum number.

Symbol	Name	related property/properties
n	principal quantum number	
l		
m_l		

12. Pay attention to which options for the quantum numbers l and m_l are available in the simulation depending on the chosen value of n. Are all combinations of n, l, and m_l possible? If not, which values of l and m_l are allowed for a given value of n?

BONUS

13. Challenge questions:

a) Define the terms "radial node" and "angular node" as they pertain to atomic orbitals.

b) Keeping the value of l constant (e.g. l=0), use Simulation C to visualize the orbitals for varying values of n. Observe the shape of each orbital. What pattern do you see?

c) Display the orbitals $1s$, $2p_z$, $3d_{xz}$ und $4f_{xz^2}$ in Simulation C and sketch them below. Discuss any patterns that you see. What is the general effect of l on the shape of the orbitals?

l = 0	l = 1	l = 2	l = 3
$1s$	$2p_z$	$3d_{xz}$	$4f_{xz^2}$