**Balloon Built Molecular Orbitals**

Objectives:

* A student should be able to build molecular orbitals resulting from combinations of atomic orbitals for homonuclear diatomic molecules
* A student should be able to visually interpret symmetry considerations of atomic orbital mixing
* A student should be able to explain differing orbital overlap resulting from p orbitals with different orientations
* A student should be able to order molecular orbitals from lowest to highest energy

Equipment:

* Two different colors of balloons, roughly 8 of each color (if you have a large class, you could blow up 16 of each color in order to allow for every MO to be formed simultaneously)

Instructions:

1. Blow up balloons
2. Select 8 volunteers from the class, 2 volunteers receive a single balloon (s orbitals and yes I know the balloons are not spherical!) and the other 6 receive one balloon of each color (p orbitals) and hold them together at the bottom of the balloon to form a p orbital.
3. Separate volunteers into atom A and atom B (I usually make O2, so Oxygen A and Oxygen B)
4. Ask atom A volunteers to arrange themselves in energy lowest to highest (usually from the front to back of the classroom along an aisle (your room layout may vary, but in a way that the whole class can see) as atomic orbitals. Have atom B match these energies in parallel about 10 or more feet apart. Also, ensure that there is a significant gap in space (energy) between the s and p orbitals, perhaps 15 feet.
5. Using the s orbitals of each atom, have the volunteers move towards each other with their balloons facing towards each other.
6. Discuss that when these two atoms come together the colors of the balloons may either be the same (constructive interference) or opposite (destructive interference),
   1. *Question: for each atom, where in reference to the balloon is the nucleus?* **In the “center” of the balloon (yes the balloon is not spherical, but we can pretend!)**
7. Have s orbital students hold their balloons of the same color pressed into each other a bit (and note how the balloon “smooshes” indicating interaction)
   1. *Question: Physical balloons have definite endpoints, what do we know about orbitals and wavefunctions?* **Orbitals are a pictorial representation of a wavefunction that denotes where electrons have a high probability of being located, but the wavefunctions go on beyond the edge of a pictured orbital**
8. Ask the students to change the bond axis orientation so that it faces towards different groups in the class so each student can peer down the internuclear axis.
   1. *Question: If we look down the internuclear axis (the axis of the “bond” forming between atoms), what type of atomic orbital does this combination of orbitals appear to be?* **An s orbital, and that is why we denote this type of molecular orbital to be sigma, σ (it is also worth noting that this designation is true regardless of the signs (colors) of the orbitals (balloons)**
   2. *Question: For this constructively interfering molecular orbital, where are electrons most likely to be found?* **In spaces between the two nuclei**
   3. *Question: Relative to the starting atomic s orbital energy, how would the constructively interfering molecular orbital energy change? Why?* **This bonding MO will be lower in energy relative to the individual s orbitals it is formed from because electrons are found most frequently between the two positively charged nuclei in the O2 molecule**
9. Switch one of the s orbital balloons with the opposite color and have the students form the destructively interfering σ\* MO
   1. *Question: Relative to the starting atomic s orbital energy, how would the destructively interfering molecular orbital energy change? Why?* **This bonding MO will be higher in energy relative to the individual s orbitals it is formed from because electrons are found most frequently in the areas on the outside the space between the two positively charged nuclei in the O2 molecule**
   2. *Question: Relative to the constructively interfering σ MO, how much higher in energy is the antibonding σ\* MO compared to the starting atomic s orbital energy? Why?* **Antibonding is more anti-bonding than bonding is bonding (ABIMABTBIB) because multiple repulsive forces are simultaneously at play in the anti-bonding orbital: (i) the electrons primarily reside outside the space between the atoms, pulling them apart and (ii) the remaining effective nuclear charges of the nuclei are electrostatically pushing the nuclei apart (often referred to as nuclear repulsion).**
10. Have the two s orbital students remain in MO positions, one holding both balloons of the s orbital bonding MO and the other holding both balloons of the antibonding MO.
11. Have students holding two opposite colored balloons (p orbitals) hold the bottom of both balloons at the center with their fingers and define x,y,z axes of the space (with z being the direction towards the other atom) and have students hold their balloons appropriately to represent px, py and pz orbitals
    1. *Question: For each atom, where in reference to the balloons is the nucleus?* **In the space between the balloons (where students fingers are holding together the two bottoms of the balloons)**
    2. *Question: Which atomic p orbitals can combine with each other to form MO’s (At this point in the course, I have not covered symmetry, so in discussions of what atomic orbitals can combine with each other to form molecular orbitals, I use the tenet that combining atomic orbitals must have the same number of lobes pointed in the same directions in order to interact (combine) and form a molecular orbital.)* **px with px, py with py, pz with pz**
12. Have the students that represent px, py, px orbitals for each atom move towards each other and interact with their partner on the other atom (preferably constructive (same color) interference)
13. Ask the pz orbital students to change the bond axis orientation so that it faces towards different groups in the class so each student can peer down the internuclear axis.
    1. *Question: If we look down the internuclear axis (the axis of the “bond” forming between atoms), what type of atomic orbital does this combination of orbitals appear to be?* **An s orbital!, and that is why we denote this type of molecular orbital to be sigma, σ, despite it being formed from p orbitals!**
14. Ask the px or py orbital students to change the bond axis orientation so that it faces towards different groups in the class so each student can peer down the internuclear axis.
    1. *Question: If we look down the internuclear axis (the axis of the “bond” forming between atoms), what type of atomic orbital does this combination of orbitals appear to be?* **A p orbital!, and that is why we denote this type of molecular orbital to be pi, π**
15. Compare the constructively interfering molecular orbitals formed form pz and px (point out and ensure that the distance between the nuclei are held constant for both molecular orbitals)
    1. *Question: Which bonding orbital do you expect to be lower in energy? Why?* **The pz bonding orbital will be lower in energy because it has greater atomic orbital overlap as the lobes are pointing out from the nuclei towards each other directly, increasing constructive interference (this will also be true for destructive interference causing it to be higher energy!)**
16. Compare the constructively interfering molecular orbitals formed form py and px
    1. *Question: Which bonding orbital do you expect to be lower in energy? Why?* **They will be equal in energy as they are exact matches of each other in terms of constructive interference, just oriented in different directions, therefore they are degenerate**
17. Ask all p orbital students to reorient their balloons to show the destructively interfering (anti-bonding) molecular orbital for both the degenerate π\* orbitals (from px and py) and the σ\* (from pz).
    1. *Question: Which anti-bonding orbital(s) will be highest in energy?* **The σ\* orbital formed from pz atomic orbitals**
18. (optional) With all 8 students each holding a newly formed molecular orbital, have the students consider how many valence electrons O2 has and how to fill in those electrons.
    1. *Question: How many total valence electrons should the molecular orbital diagram of O2 have?* **12 valence electrons**
    2. *Question: Filling in electrons following Hund’s rule (Every orbital in a sublevel is singly occupied before any orbital is doubly occupied. All of the electrons in singly occupied orbitals have the same spin), which orbital(s) will be the frontier orbitals?* **The antibonding π\* orbitals formed from px and py orbitals each have one electron, both with the same spin**
    3. *Question: Is O2 diamagnetic or paramagnetic?* **Paramagnetic**
19. (Optional) Have a student that represented an atomic s orbital on one atom and the atomic pz orbital on the other atom bring their orbitals together.
    1. *Question: From the perspective of peering down the internuclear axis, does a pz orbital have a different profile or appearance than an s orbital?* **No**
20. Indeed, a full analysis of even a molecule as simple as O2 should incorporate the combinations of ALL orbitals with equivalent “symmetry” and these interaction CAN change the ordering of orbital energies that we derived and for all homonuclear diatomics prior to O2 the bonding π orbitals formed from px and py atomic orbitals lie lower in energy than the bonding σ orbital formed from pz atomic orbitals.

Note: At this point in the course, I have not covered symmetry, so in discussions of what atomic orbitals can combine with each other to form molecular orbitals, I use the simplified principle that combining atomic orbitals must have the same number of lobes pointed in the same directions in order to interact (combine) and form a molecular orbital.

Note also that in this activity that we are simplifying reality a bit by not accounting for the fact that pz orbitals and s orbitals on both atoms can contribute, but this can be discussed optionally at the end of the activity as shown.

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