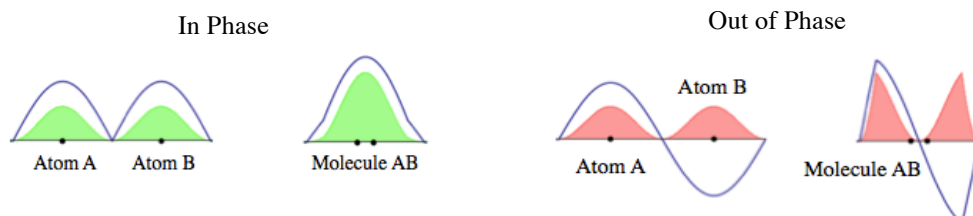


## 25. Correlation Diagrams

The bonding of molecules occurs when electron clouds, or orbitals\*, interfere between two atoms. Within this structure, the two or more atomic orbitals change to become a set of molecular orbitals. The number of atomic orbitals is the same as the number of molecular orbitals that are created in bonding. The diagrams below show two atomic orbitals before interfering and the resulting molecular orbital.



As stated above, we know that if there are two initial atomic electron orbitals, there must be two resulting molecular orbitals. As a result, two interfering waves will result in two molecular orbitals: one from in phase waves, and one from out of phase waves (both of the images above).

1) If atoms A and B can hold two electrons each, how many molecular orbitals must be created to accommodate these four electrons?

2) Compare the wavelengths of the following waves pictured above:

- the atomic 1s orbital (Atom A)
- the in-phase molecular orbital (molecule AB on the left above)
- the out-of-phase molecular orbital (molecule AB on the right above)

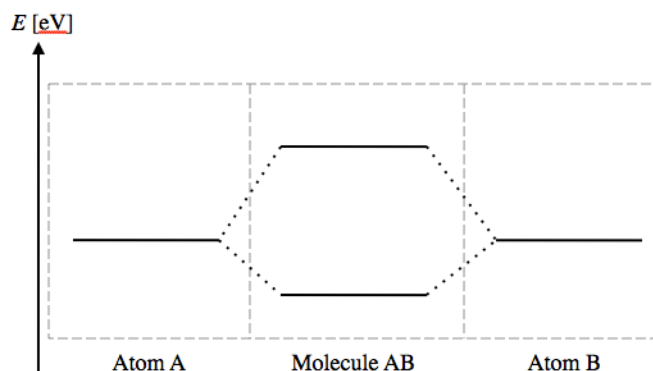
Which one has the largest wavelength? the smallest?

3) Based on what we learned about the relationship between the wavelength of a standing wave and the energy of a standing wave (de Broglie / particle-in-a-box), which of the three orbitals is the highest energy? the lowest?

\*Note: here we use the term *orbitals* to mean 3D electron clouds

Correlation diagrams show energy diagrams of the original electron orbitals and the resulting molecular orbitals. The correlation diagram below shows an example of atom A and atom B combining into molecule AB. By including the individual atoms and the molecules on the same diagram the change in energy of the orbitals can be compared.

4) Based on your answers in the previous sections, label the molecule orbital energies in the diagram to the right as either in phase electron wave interference or out of phase electron wave interference. Explain your choice.



5) Label each of the molecular orbitals as either “bonding” or “anti-bonding”. Explain your answer.

\*Note: here we use the term *orbitals* to mean 3D electron clouds