1 The kinetic energy of the antibonding combination of a pair of AO's is ...

- A greater than that for the bonding combination
- B about the same that for the bonding combination
- C less than that for the bonding combination

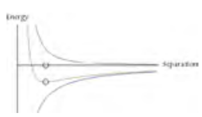
2 The total energy of the antibonding combination of a pair of AO's is ...

- A never negative
- B has a minimum near the bond distance
- C about the same as for the bonding combination
- D is smaller the larger the separation
- E A and D

3 The potential energy of the antibonding combination of a pair of AO's is ...

- A never negative
- B about zero
- C about the same as for the bonding combination

4 As a pair of atoms approach from a large separation, initially the total energy of the MO resulting from in-phase overlap of their AO's ...



- A goes up, due to increased kinetic energy.
- B goes down, due to enhancement of electron density between the atoms.
- C goes up, due to depletion of electron density between the atoms.
- D None of the above

5 As a pair of atoms approach from a large separation, initially the total energy of the MO resulting from out-of-phase overlap of their AO's ...

- A goes down, due to decreased kinetic energy.
- B goes down, due to enhancement of electron density between the atoms.
- C goes up, due to depletion of electron density between the atoms.
- D None of the above

6 A pair of atoms approach from a large separation, and the resulting MO has equal in-phase and out-of-phase overlap of their AO's. The result is that initially the total energy ...

- A goes up, due to increased kinetic energy.
- B goes down, due to enhancement of electron density between the atoms.
- C goes up, due to depletion of electron density between the atoms.
- D None of the above

7 If AO's have only in-phase or only out-of-phase overlap, we say they have correct symmetry. If AO's have equal amounts of in-phase and out-of-phase overlap, we say they have incorrect symmetry. Which pairs of AO's on different atoms have correct symmetry?

- A 1s + 1s
- B 1s + 2s
- C both
- D neither

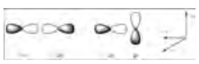
8 Which pairs of AO's on different atoms have correct symmetry? Assume z is along bond axis.

A 1s + 2pz
B 1s + 2py
C both
D neither

9 Which pairs of AO's on different atoms have correct symmetry? Assume z is along bond axis.

A 2s + 2pz
B 2s + 2py
C both
D neither

10 Which pairs of AO's on different atoms have correct symmetry? Assume z is along bond axis.



A 2pz + 2pz
B 2pz + 2py
C both
D neither

11 Which pairs of AO's on different atoms have correct symmetry? Assume z is along bond axis.

A 2px + 2py
B 2px + 2px
C both
D neither

12 If AO's have correct symmetry, then we consider next how much they overlap. Arrange the pairs of AO's in Li2 according to increasing overlap when the atoms are at the lowest energy separation (the bond length).

A 1s + 1s < 2s + 2s < 1s + 2s
B 1s + 2s < 1s + 1s < 2s + 2s
C 1s + 1s < 1s + 2s < 2s + 2s

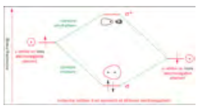
13 Finally, once we know the pair of AO's with correct symmetry and greatest overlap, we consider relative AO energies. The bonding/antibonding effect will be greatest for AO's closest in energy. Arrange the pairs of AO's in Li2 according to increasing energy change at the bond length.

A 1s + 1s < 2s + 2s < 1s + 2s
B 1s + 2s < 1s + 1s < 2s + 2s
C 1s + 1s < 1s + 2s < 2s + 2s

14 Which pair of AO's in HF will interact most strongly? Assume z is along the bond axis.

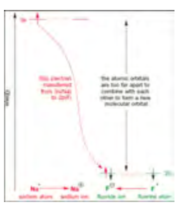
A H 1s + F 1s
B H 1s + F 2s
C H 1s + F 2pz
D H 1s + F 2py
E C and D

15 Assume AO1 and AO2 have correct relative symmetry, greatest overlap, and are closest in energy. AO1 has IE = 5 eV and AO2 has IE = 6 eV. Which of the following is true?



- A Bonding MO has more AO1 than AO2
- B Bonding MO has more AO2 than AO1
- C Antibonding MO is almost entirely AO1
- D Antibonding MO is almost entirely AO2
- E A and D

16 AO1 has IE = 3 eV and AO2 has IE = 12 eV. Which of the following is true?



- A Bonding MO is almost entirely AO1
- B Bonding MO is has a little more AO2 than AO1
- C Antibonding MO is almost entirely AO1
- D Antibonding MO has a little more AO1 than AO2
- E None of the above

17 The bond pair in Na:F is in the Na 3s + F 2pz MO. The bond pair in H:F is in the H 1s + F 2pz MO. Which of the following is true?

- A The bond pair is almost entirely on the F of HF.
- B The bond pair is almost entirely on the H of HF.
- C The bond pair is almost entirely on the F of NaF.
- D The bond pair is almost entirely on the Na of NaF.
- E A and D

18 Na 3s has IE = 5.1 eV. H 1s has IE = 13.6 eV. F has IE = 17.4 eV. NaF is more ionic than HF because ...

- A Na 3s has lower IE than does H 1s
- B F 2pz has higher IE than does H 1s
- C Na 3s has lower IE than does F 2pz
- D F 2pz has higher IE than does Na 3s

19 We learn that it is the valence electrons on different atoms that interact with one another, rather than the core electrons. What is the best explanation for this.

- A Adjacent valence electron waves have the greatest in-phase or out-of-phase overlap.
- B Adjacent valence electron waves have the same energy.
- C Core electron clouds have the wrong symmetry.
- D Core electron clouds move with the wrong frequency.