Questions on Symmetry, Overlap, Energy

CH101 Fall 2015
Boston University

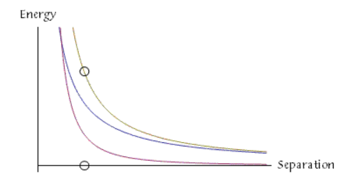
BOSTON UNIVERSITY

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

33% 1. greater than that for the bonding combination

33% 2. about the same that for the bonding combination

33% 3. less than that for the bonding combination



BOSTON UNIVERSITY Response Counter 10 2

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

20% 1. never negative

20% 2. has a minimum near the bond distance

20% 3. about the same as for the bonding combination

20% 4. is smaller the larger the separation

20% 5. 1 and 4

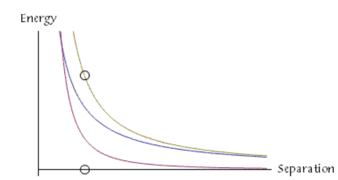
BOSTON UNIVERSITY Response Counter 10 3

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

33% 1. never negative

33% 2. about zero

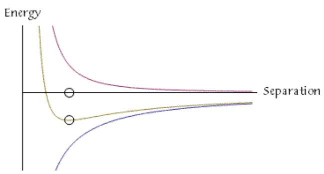
33% 3. about the same as for the bonding combination



BOSTON UNIVERSITY Response Counter 10 4

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 ...

25% 1. goes up, due to increased kinetic energy.
25% 2. goes down, due to enhancement of electron density between the atoms
25% 3. goes up, due to depletion of electron density between the atoms
25% 4. None of thes3

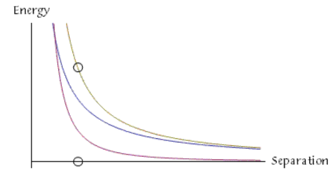


BOSTON UNIVERSITY Response Counter 10 5

Questions on SOE: Symmetry, Overalp, Energy Copyright © 2015 Dan Dill dan@bu.edu

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 ...

25% 1. goes down, due to decreased kinetic energy
25% 2. goes down, due to enhancement of electron density between the atoms
25% 3. goes up, due to depletion of electron density between the atoms
25% 4. None of thes3



BOSTON UNIVERSITY Response Counter 10 6

Questions on SOE: Symmetry, Overalp, Energy Copyright © 2015 Dan Dill dan@bu.edu

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** ...

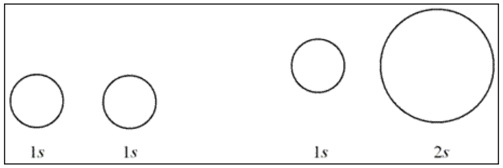
25% 1. goes up, due to increased kinetic energy
25% 2. goes down, due to enhancement of electron density between the atoms
25% 3. goes up, due to depletion of electron density between the atoms
25% 4. None of these

BOSTON UNIVERSITY Response Counter 10 7

Questions on SOE: Symmetry, Overalp, Energy Copyright © 2015 Dan Dill dan@bu.edu

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**?

25% 1. 1s and 1s
25% 2. 1s and 2s
25% 3. both
25% 4. neither

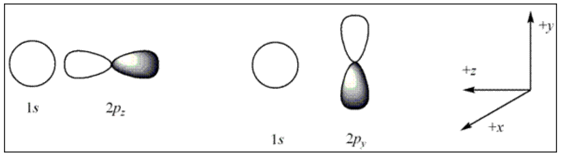


BOSTON UNIVERSITY Response Counter 10 8

Qeustions on SOE: Symmetry, Overalp, Energy

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

25% 1. 1s and $2p_z$
25% 2. 1s and $2p_y$
25% 3. both
25% 4. neither



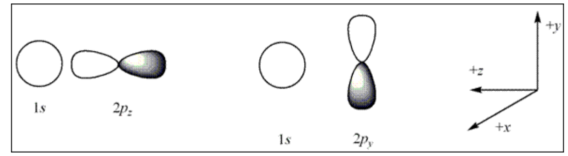
Response Counter

10 9

Qeustions on SOE: Symmetry, Overalp, Energy

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

25% 1. 2s and $2p_z$
25% 2. 2s and $2p_y$
25% 3. both
25% 4. neither



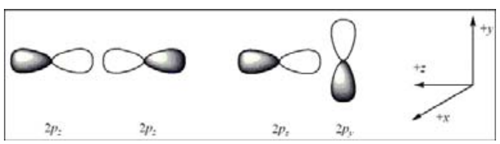
Response Counter

10 10

Qeustions on SOE: Symmetry, Overalp, Energy

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

25% 1. $2p_z$ and $2p_z$
25% 2. $2p_z$ and $2p_y$
25% 3. both
25% 4. neither



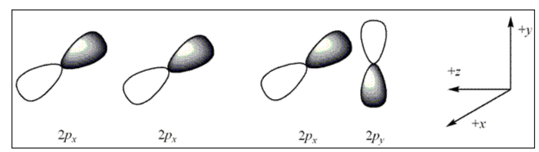
Response Counter

10 11

Qeustions on SOE: Symmetry, Overalp, Energy

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

25% 1. $2p_x$ and $2p_z$
25% 2. $2p_x$ and $2p_x$
25% 3. both
25% 4. neither



Response Counter

10 12

12. If AO's have correct symmetry, then we consider next how much they overlap. Arrange the pairs of AO's in Li_2 according to **increasing overlap** when the atoms are at the lowest energy separation (the bond length)

33% 1. 1s + 1s < 2s + 2s < 1s + 2s

33% 2. 1s + 2s < 1s + 1s < 2s + 2s

33% 3. 1s + 1s < 1s + 2s < 2s + 2s

BOSTON UNIVERSITY Response Counter 10 13

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 Li_2 according to **increasing energy change** at the bond length

33% 1. 1s + 1s < 2s + 2s < 1s + 2s

33% 2. 1s + 2s < 1s + 1s < 2s + 2s

33% 3. 1s + 1s < 1s + 2s < 2s + 2s

BOSTON UNIVERSITY Response Counter 10 14

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

20% 1. H 1s + F 1s

20% 2. H 1s + F 2s

20% 3. H 1s + F $2p_z$

20% 4. H 1s + F $2p_y$

20% 5. 3 and 4

BOSTON UNIVERSITY Response Counter 10 15

15. Assume AO_1 and AO_2 have correct relative symmetry, greatest overlap, and are closest in energy. **AO_1 has *IE* = 5 eV** and **AO_2 has *IE* = 6 eV**. Which of the following is true?

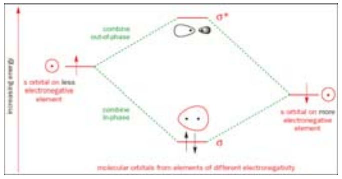
20% 1. Bonding MO has more AO_1 than AO_2

20% 2. Bonding MO has more AO_2 than AO_1

20% 3. Antibonding MO is almost entirely AO_1

20% 4. Antibonding MO is almost entirely AO_2

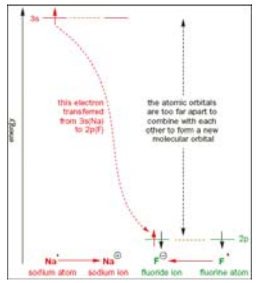
20% 5. 1 and 4



BOSTON UNIVERSITY Response Counter 10 16

16. **AO_1 has *IE* = 3 eV** and **AO_2 has *IE* = 12 eV**. Which of the following is true?

20% 1. Bonding MO is almost entirely AO_1
20% 2. Bonding MO is has a little more AO_2 than AO_1
20% 3. Antibonding MO is almost entirely AO_1
20% 4. Antibonding MO has a little more AO_1 than AO_2
20% 5. None of the above



BOSTON UNIVERSITY Response Counter

10 17

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

20% 1. The bond pair is almost entirely on the F of HF.
20% 2. The bond pair is almost entirely on the H of HF.
20% 3. The bond pair is almost entirely on the F of NaF.
20% 4. The bond pair is almost entirely on the Na of NaF.
20% 5. 1 and 4

BOSTON UNIVERSITY Response Counter

10 18

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

25% 1. Na 3s has lower *IE* than does H 1s
25% 2. F $2p_z$ has higher *IE* than does H 1s
25% 3. Na 3s has lower *IE* than does F $2p_z$
25% 4. F $2p_z$ has higher *IE* than does Na 3

BOSTON UNIVERSITY Response Counter

10 19

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?

25% 1. Valence electron AOs have the greatest in-phase or out-of-phase overlap.
25% 2. Valence electron AOs have the same energy.
25% 3. Core electron AOs have the wrong symmetry.
25% 4. Core electron AOs are filled with electrons

BOSTON UNIVERSITY Response Counter

10 20

