

Lecture 38 CH101 A2 (MWF 11:15 am) Fall 2018 Copyright © 2018 Dan Dill dan@bu.edu

[TP] In the  $\text{HO}^-$  correlation diagram, the O 2s AO is nonbonding because ...

25% 1. it has no net overlap with the H 1s AO  
 25% 2. It has the wrong symmetry  
 25% 3. it has a lower ionization energy than the O 2p AOs  
 25% 4. it has a larger  $Z_{\text{eff}}$  than the O 2p AOs

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Response Counter 10 1

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 Wednesday, December 12, 2018

For today:

- Course evaluation
- MO description of hydroxide ( $\text{OH}^-$ ) and HOH (water)

Next lecture: CH101 Spring 2019: Accounting for central atom geometry

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### Course evaluation

<https://bu.campuslabs.com/courseeval>

- Lecture, discussion, and lab
- Your responses are anonymous.
- They will be read many people.
- The more thoughtful your responses, the more helpful they will be.
- If more time is needed, you may continue until December 16.

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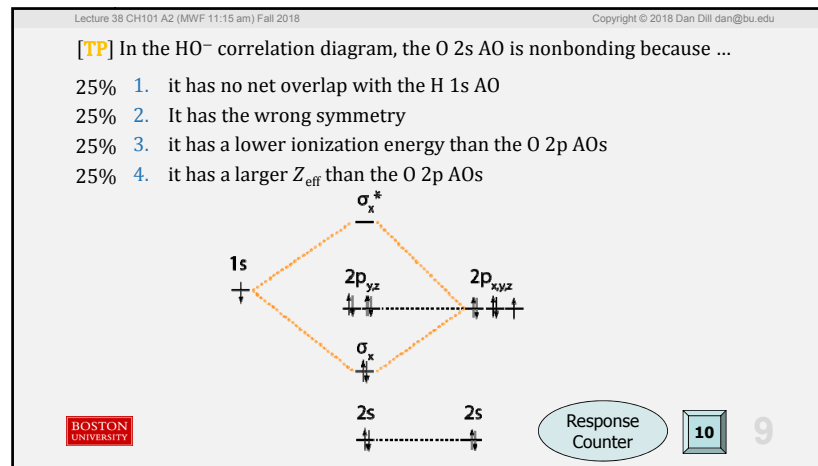
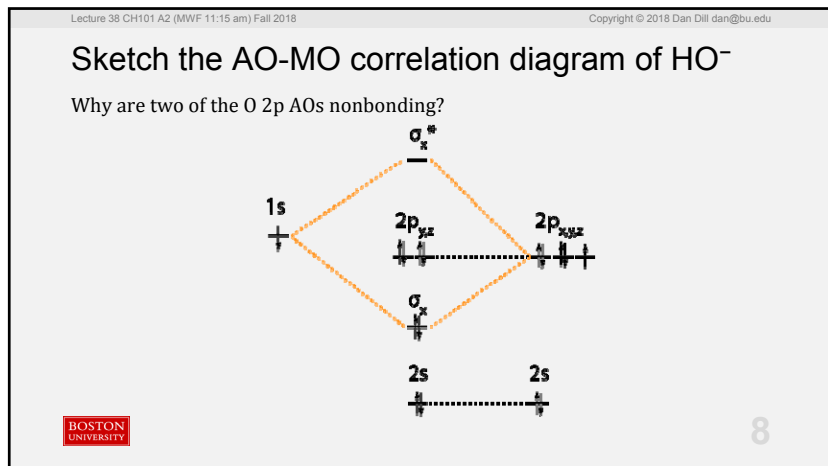
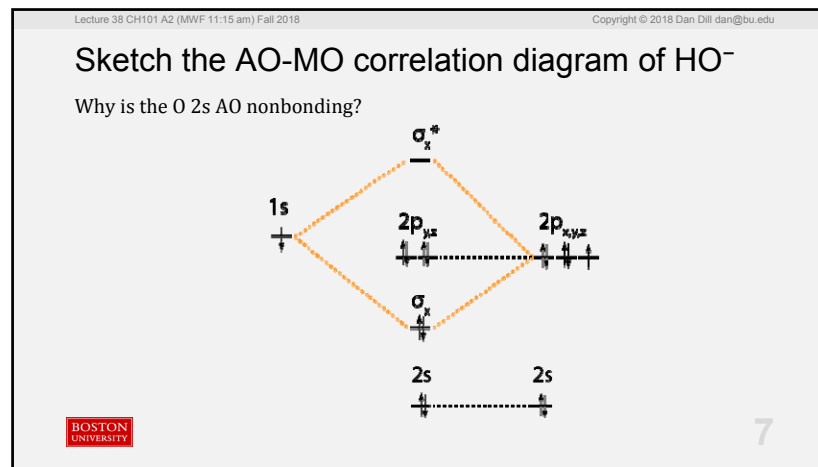
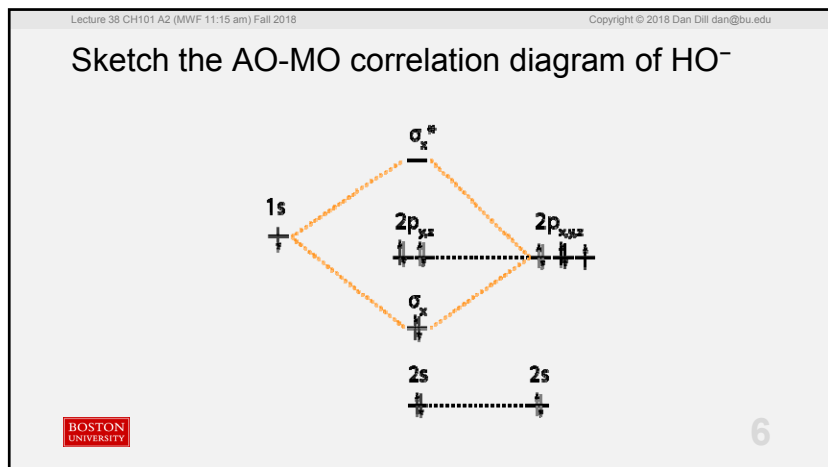
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### Sketch the AO-MO correlation diagram of $\text{HO}^-$

Note:  $IE_{\text{O}} > IE_{\text{H}}$

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**[Quiz]** In the HO<sup>-</sup> correlation diagram, the two O 2p AOs are nonbonding because ...

33% 1. they have no net overlap with the H 1s AO (incorrect symmetry)

33% 2. they have a higher ionization energy than the H 1s AO

33% 3. they have a larger Z<sub>eff</sub> than the the H 1s AO

The diagram shows the energy levels for HO<sup>-</sup>. On the left is a single H 1s orbital with one electron. On the right are O 2s and two O 2p orbitals (2p<sub>yz</sub> and 2p<sub>xz</sub>), each with two electrons. The resulting MOs are a bonding sigma<sub>x</sub> orbital (filled with two electrons) and an antibonding sigma<sub>x</sub>\* orbital (empty). The two O 2p orbitals remain nonbonding at their original energy level.

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### Sketch the AO-MO correlation diagram of HOH

Hint: Represent the second H as an additional 1s AO

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### Sketch the AO-MO correlation diagram of HOH

Hint: Represent the second H as an additional 1s AO

The diagram shows the energy levels for HOH. On the left are two H 1s orbitals, each with one electron. On the right are O 2s and two O 2p orbitals (2p<sub>z</sub> and 2p<sub>xz</sub>), each with two electrons. The resulting MOs are a bonding sigma<sub>x</sub> sigma<sub>y</sub> orbital (filled with two electrons) and an antibonding sigma<sub>x</sub>\* sigma<sub>y</sub>\* orbital (empty). The two O 2p orbitals remain nonbonding.

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**[Group Quiz]** Based on the AO-MO correlation diagram of HOH, the H-O-H bond angle must be ...

0% 1. 90°

0% 2. 109°

0% 3. 120°

0% 4. 180°

The diagram shows the energy levels for HOH. On the left are two H 1s orbitals, each with one electron. On the right are O 2s and two O 2p orbitals (2p<sub>z</sub> and 2p<sub>xz</sub>), each with two electrons. The resulting MOs are a bonding sigma<sub>x</sub> sigma<sub>y</sub> orbital (filled with two electrons) and an antibonding sigma<sub>x</sub>\* sigma<sub>y</sub>\* orbital (empty). The two O 2p orbitals remain nonbonding.

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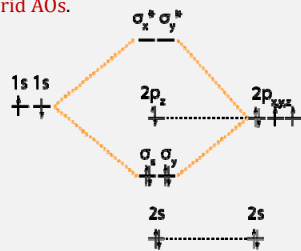
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## Sketch the AO-MO correlation diagram of HOH

Based on the AO-MO correlation diagram of HOH, the H-O-H bond angle **must be 90°**.

Our first task in **CH102 Spring 2019** is to account for the observed bond angle of ~109° by using **hybrid AOs**.

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## Until then ...

... very best wishes for your semester break.

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