Hybridization

Part 1

Reading: Gray: (4-1), (4-2), and (4-4)
OGN: (16.2)

The story so far:

MO-LCAO works great for diatomic molecules!

But...

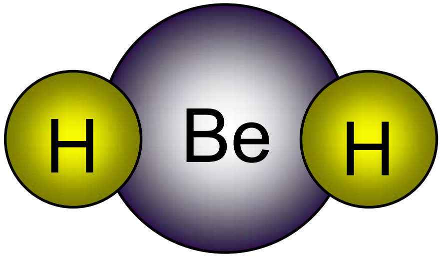
What about other numbers of atoms?

Will MO-LCAO work for polyatomic molecules?

Let's try BeH_2

We know:

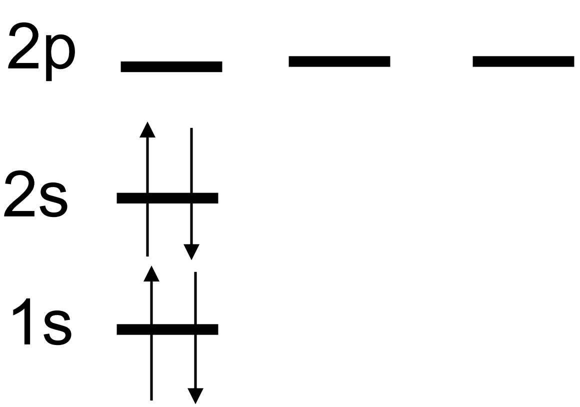
- BeH_2 is a linear molecule, by VSEPR.



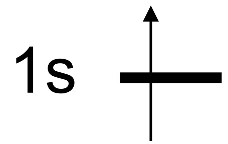
Bond angle: 180°

- The electron configuration of BeH_2 is

Be: $1s^2\ 2s^2$



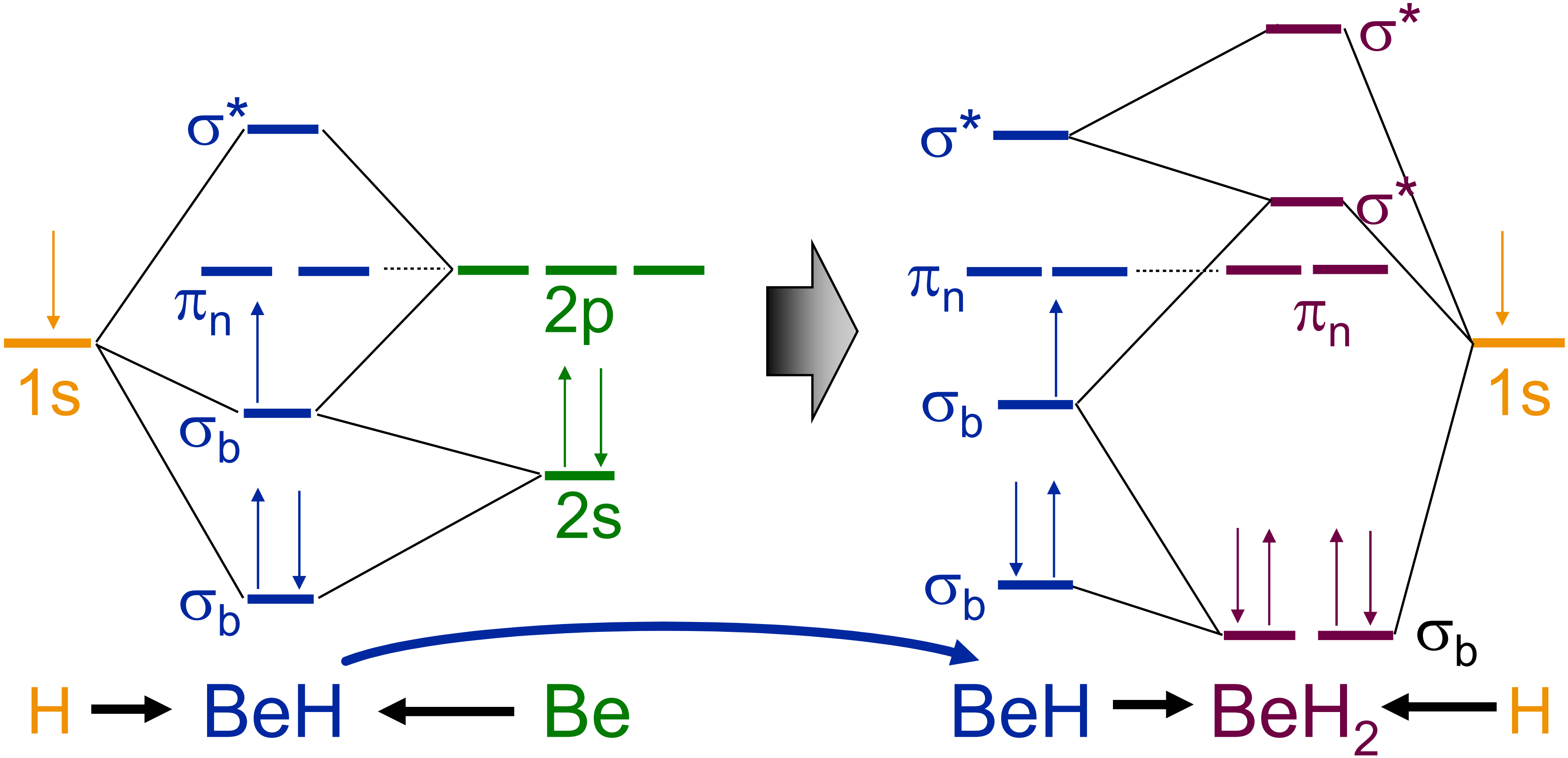
H: $1s^1$



Make MO's:

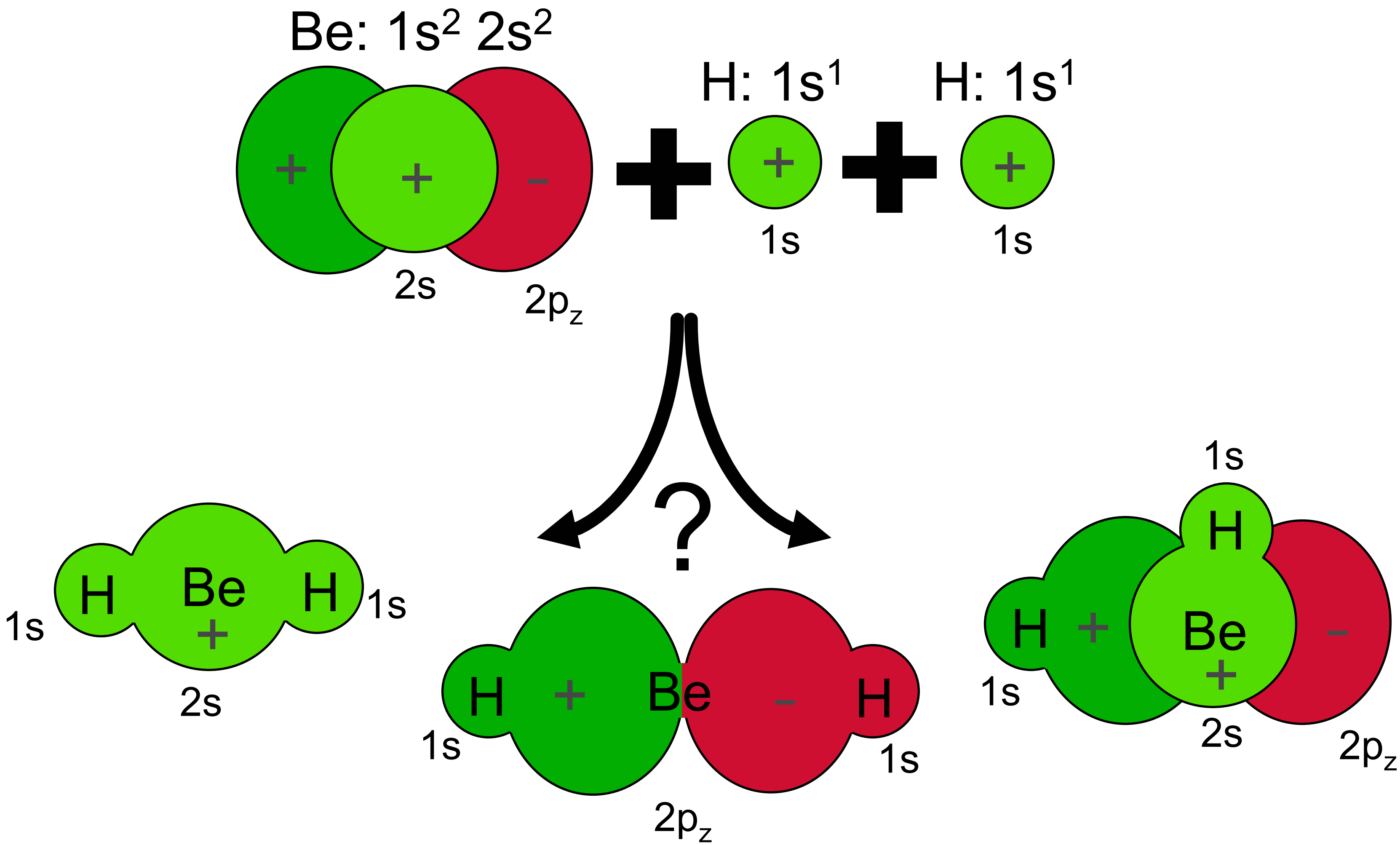
First bond **H** and **Be** to form **BeH**

Next bond **H** and **BeH** to form **BeH$_2$**



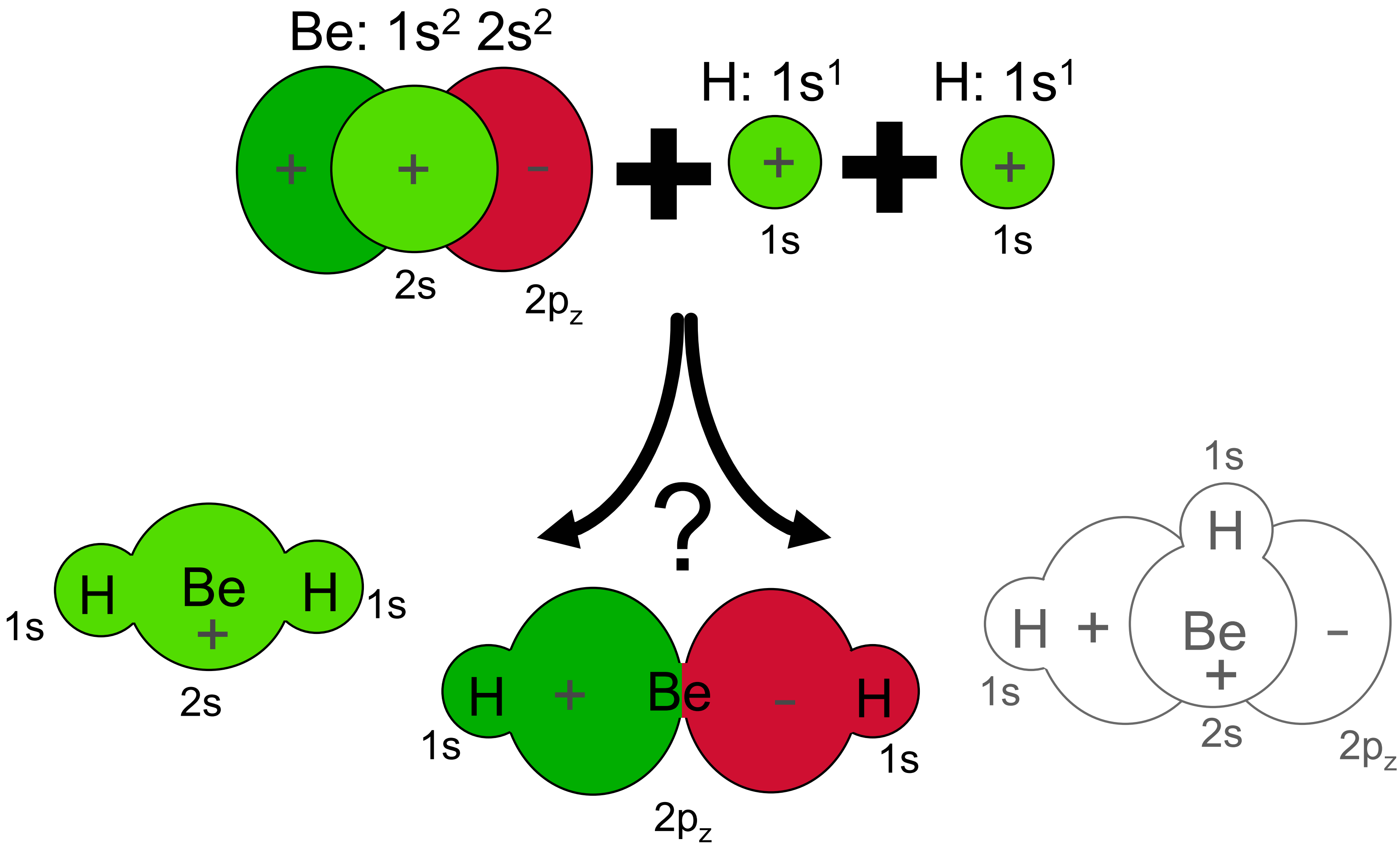
The MO's for BeH$_2$ are complicated and hard to work with.

Attempt to make a graphical model of BeH_2:



Are any of these models reasonable?

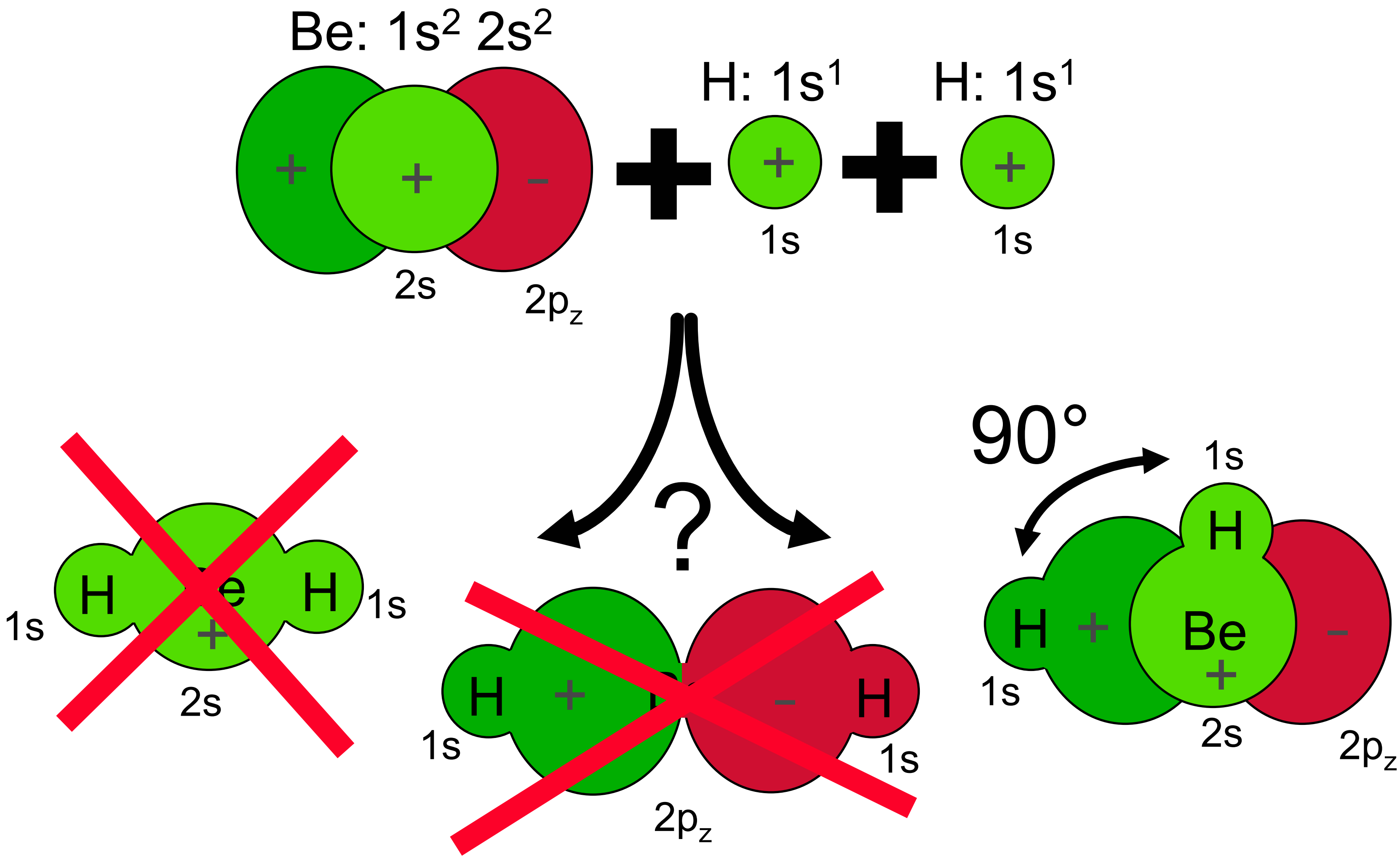
Attempt to make a graphical model of BeH_2:



These two are no good:

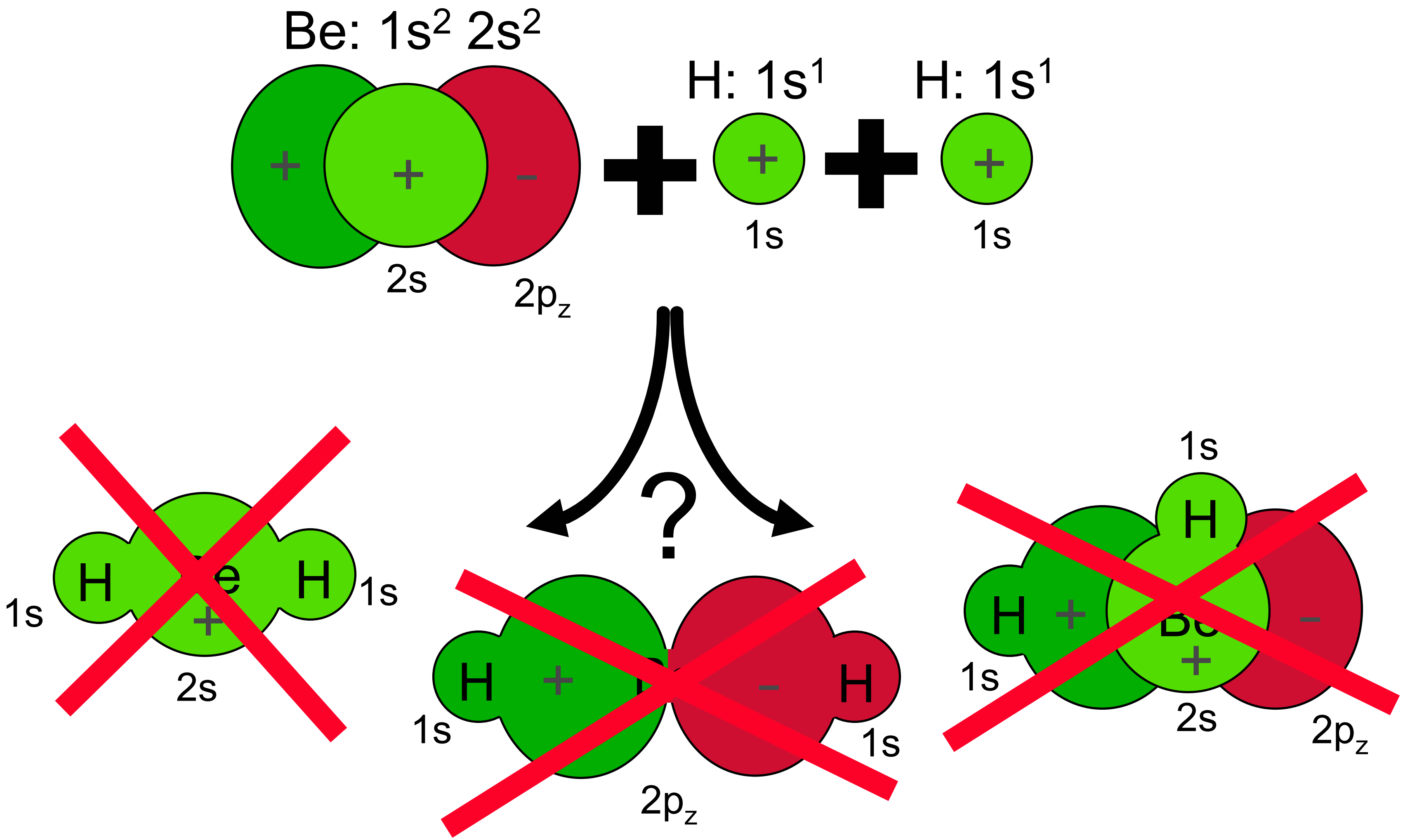
One orbital can't hold four electrons

Attempt to make a graphical model of BeH_2:



This one is no good:
According to VSEPR, the bond angle should be 180°.

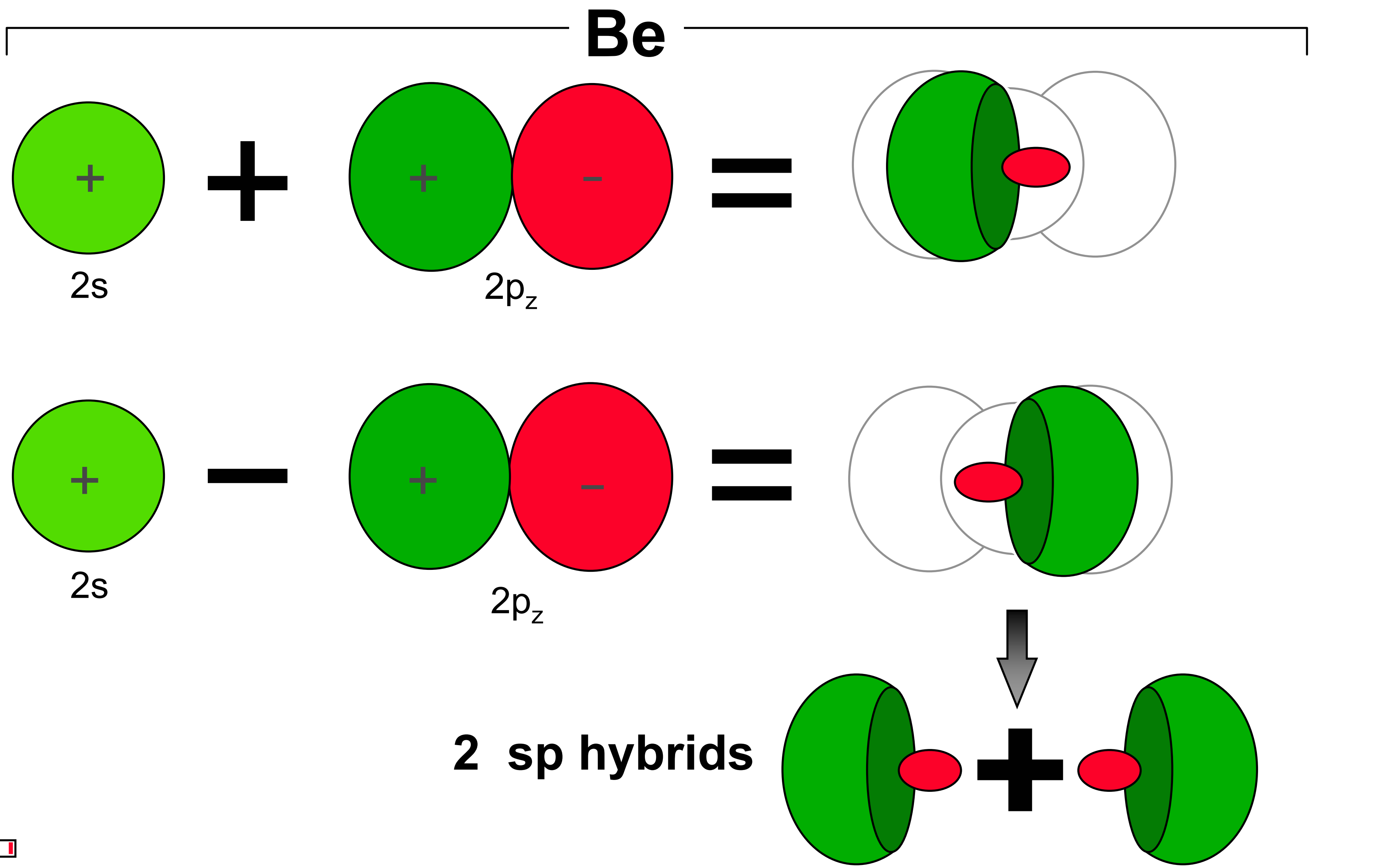
Attempt to make a graphical model of BeH_2:



Unfortunately, <u>none</u> of these models make sense.

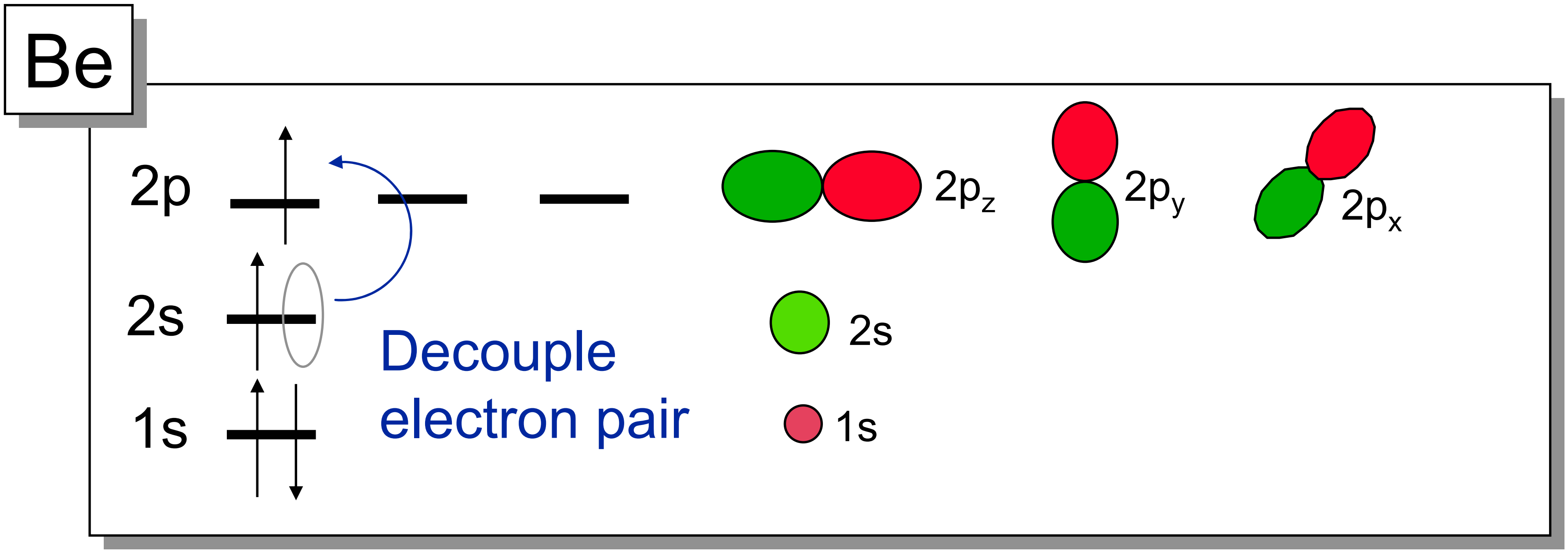
hybridized the orbitals...

Maybe if we ~~blended the orbitals together~~...



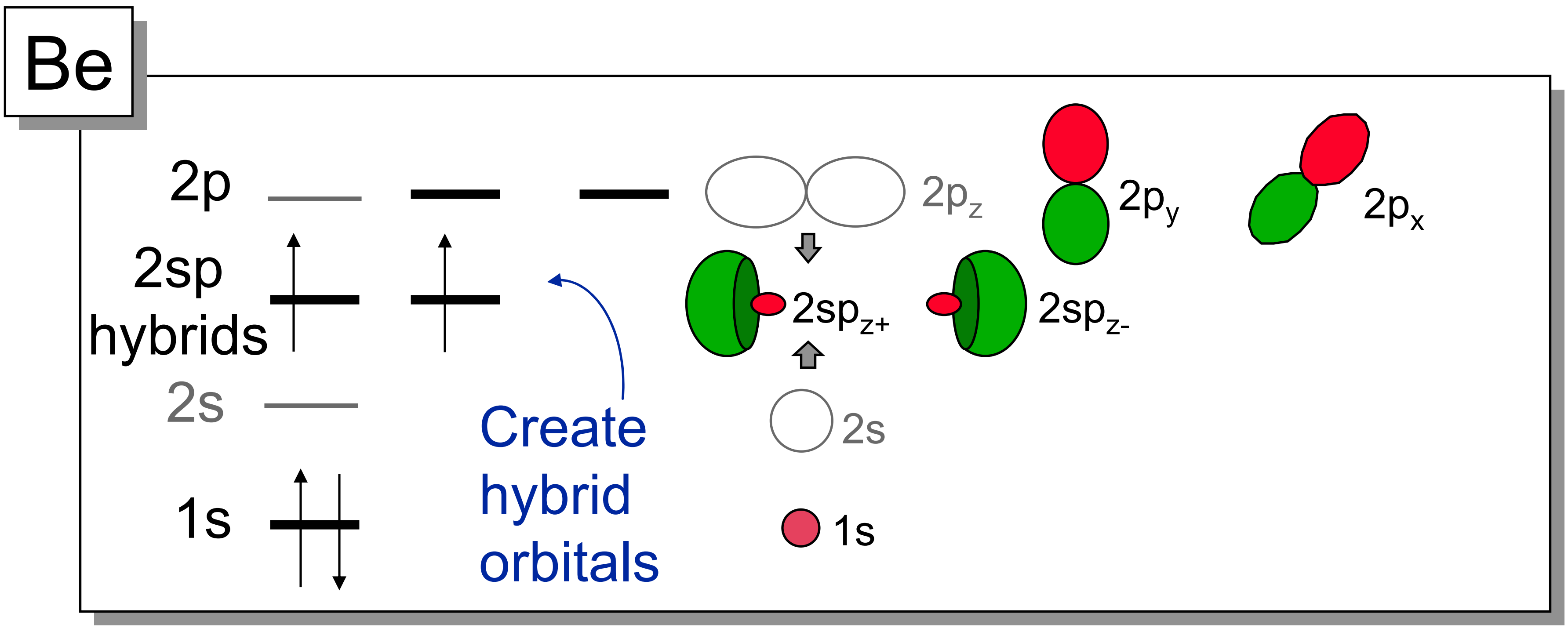
Hybridization in terms of electron configuration:

Unhybridized



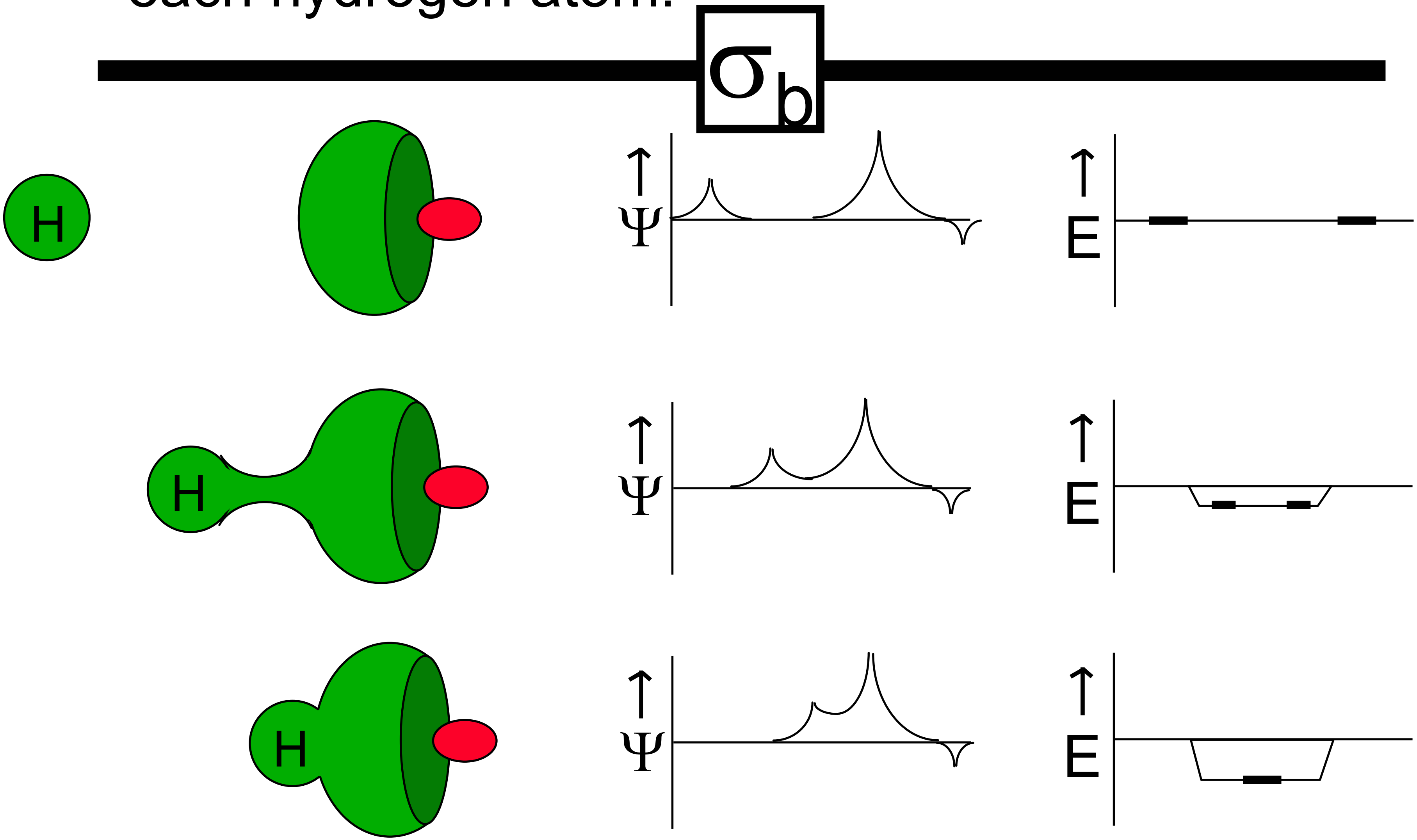
Hybridization in terms of electron configuration:

Hybridized



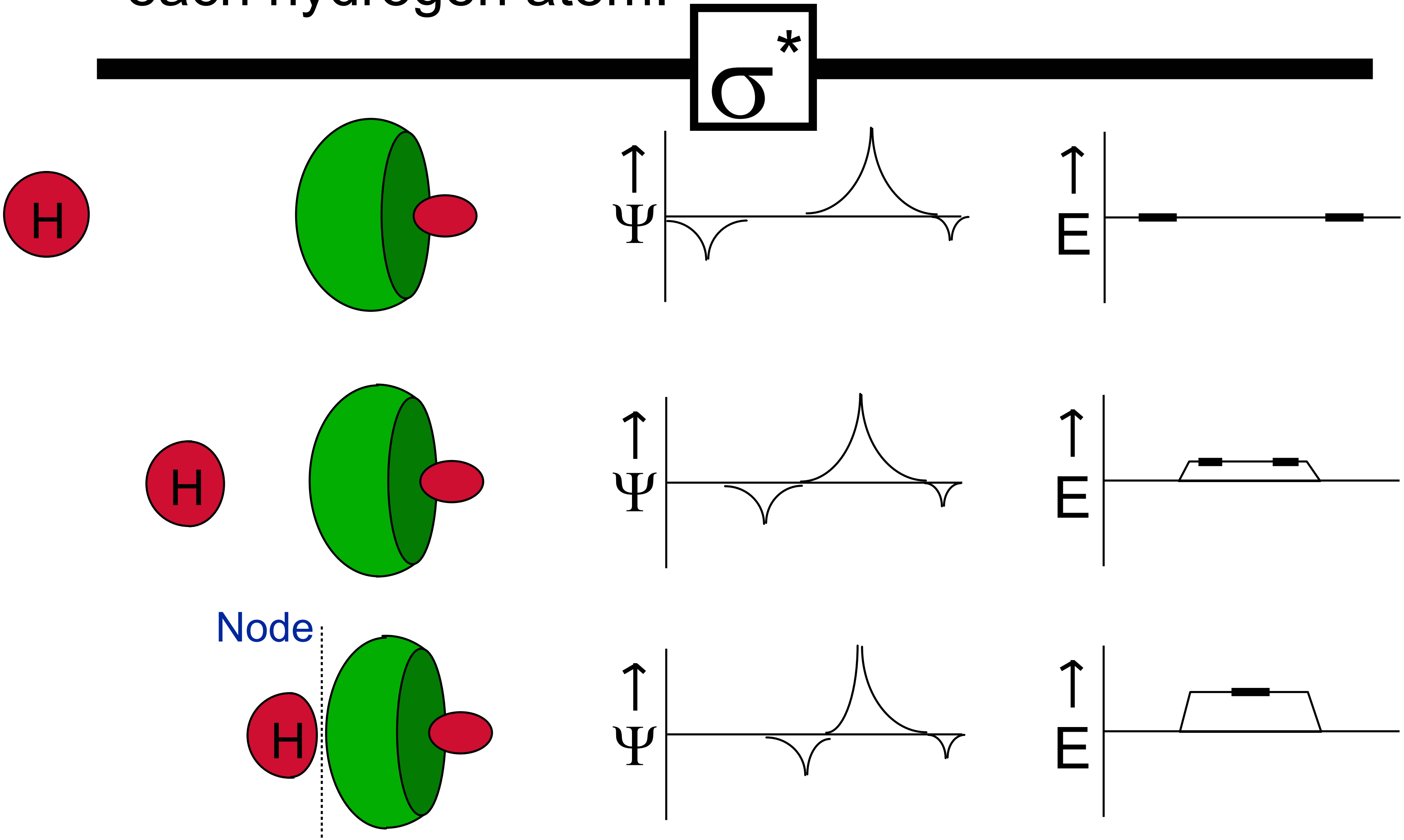
Bonding with a Hybrid Orbital:

The sp hybrids act individually to form MO's with each hydrogen atom:

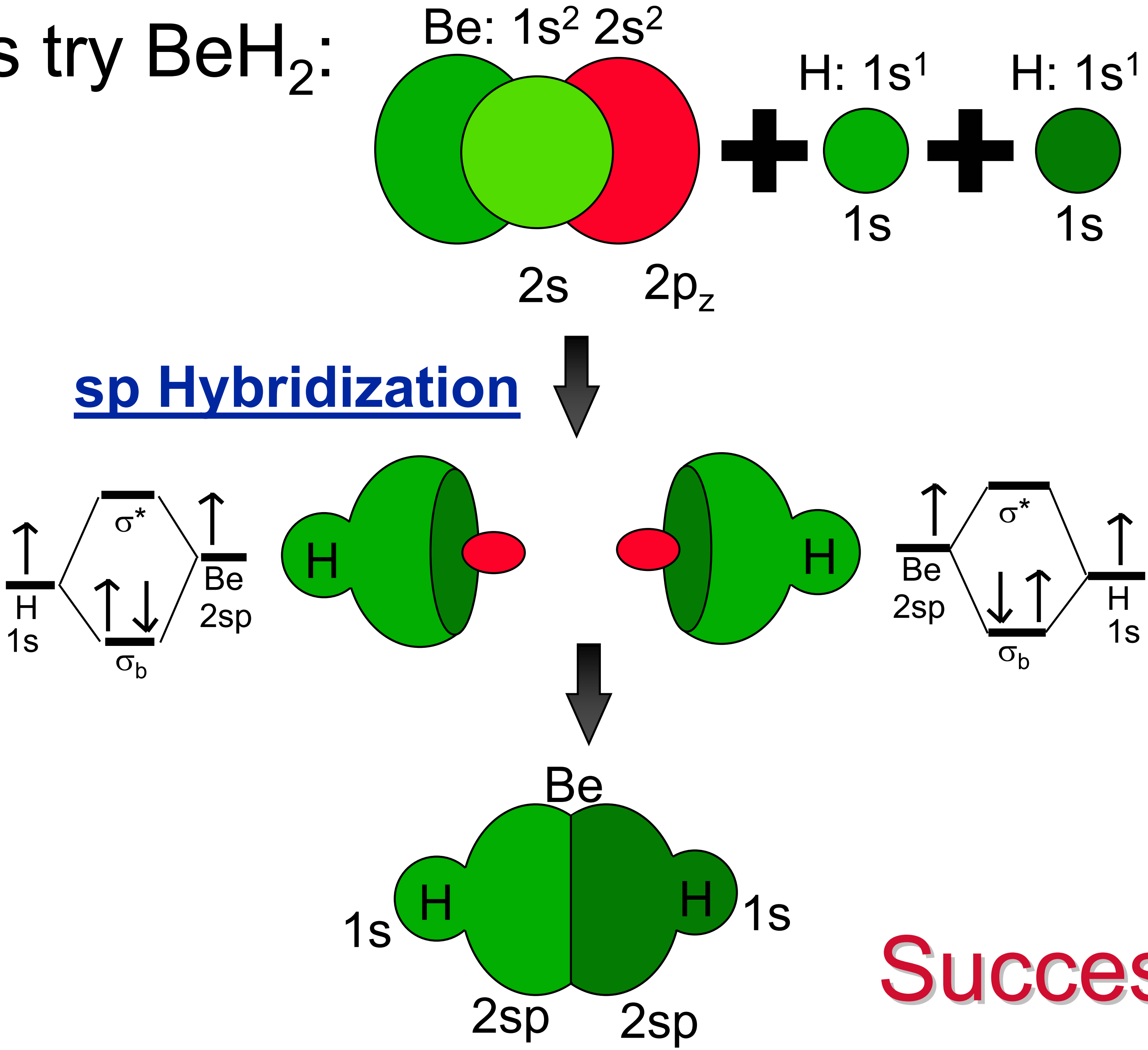


Bonding with a Hybrid Orbital:

The sp hybrids act individually to form MO's with each hydrogen atom:



Let's try BeH_2:



sp Hybridization

Success!

Rules for Hybridization Example: BeH_2

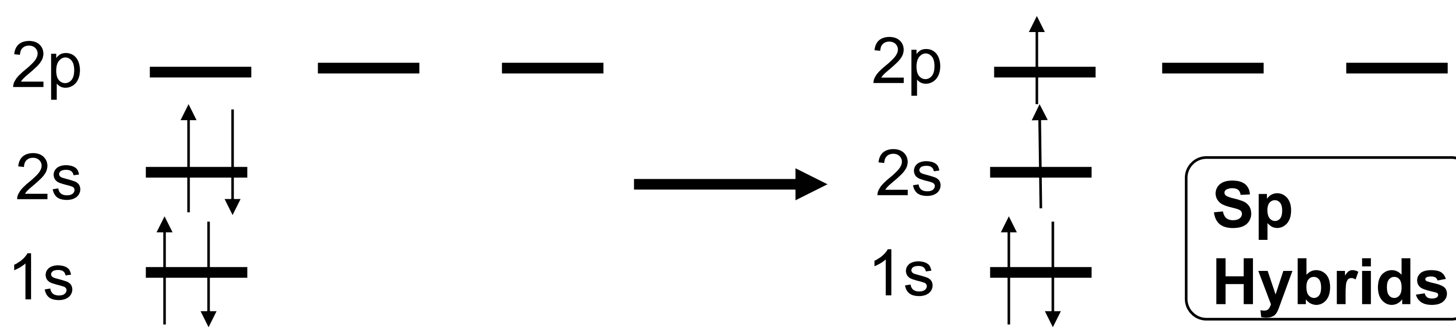
1) Assign Geometry Using VSEPR Theory

BeH_2 SN = 2 Geometry: Linear

2) Write electronic configuration of the atom to be hybridized

Be: $(1s)^2\ (2s)^2\ (2p)^0$

3) Draw energy diagram for said atom and "decouple" paired electrons



Sp Hybrids

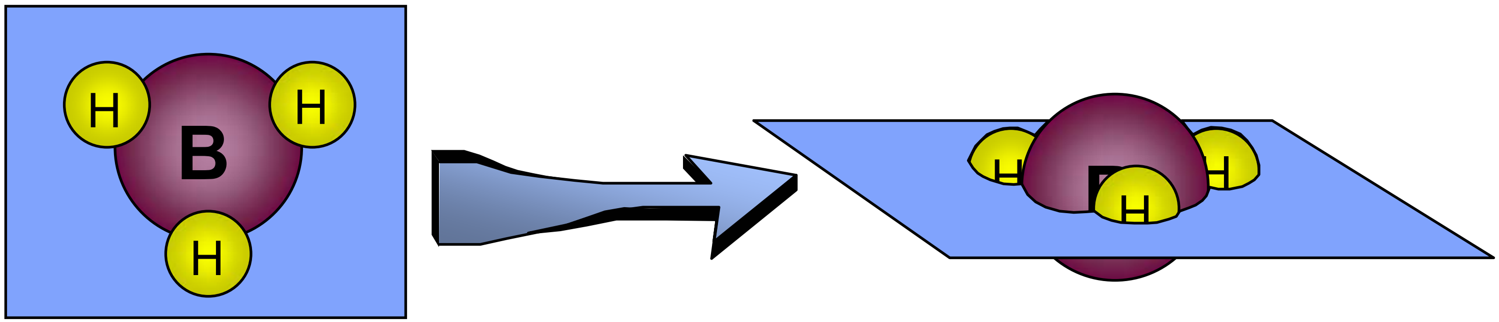
Rules for Hybridization
Example: BeH_2

4) Take linear combinations of the atomic orbitals participating in the bond to make hybrid orbitals
5) Combine hybrid orbitals with other atom's orbitals using diatomic MO theory

Make BH_3:

We know:

- The geometry, from VSEPR:

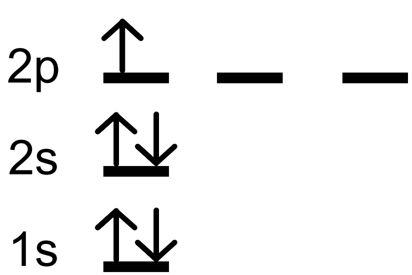


Trigonal Planar

Bond angle: 120°

- The electron configurations:

B: $1s^2\ 2s^2\ 2p^1$

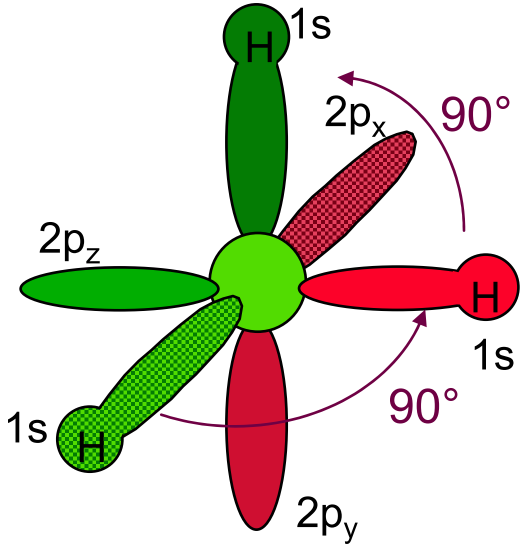


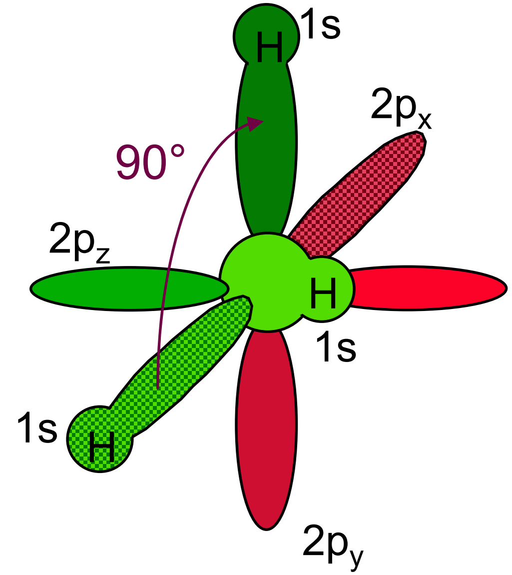
H: $1s^1$

Make BH_3:

What does this look like in terms of orbitals?

Possibilities:





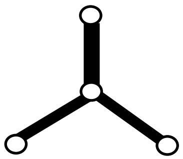
WRONG: These shapes don't match those predicted by VSEPR.

Use what we learned about hybrids:

BH_3

1) Assign Geometry Using VSEPR:

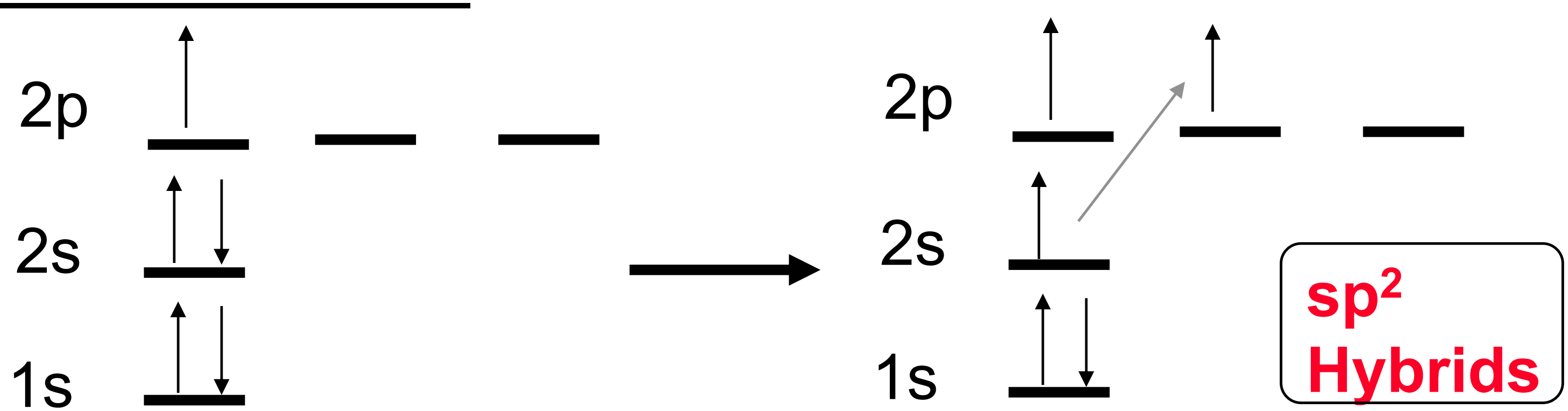
BH_3 SN = 3 Geometry: Trigonal planar



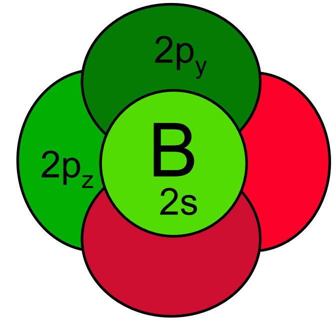
2) Write electron configuration of atom to be hybridized:

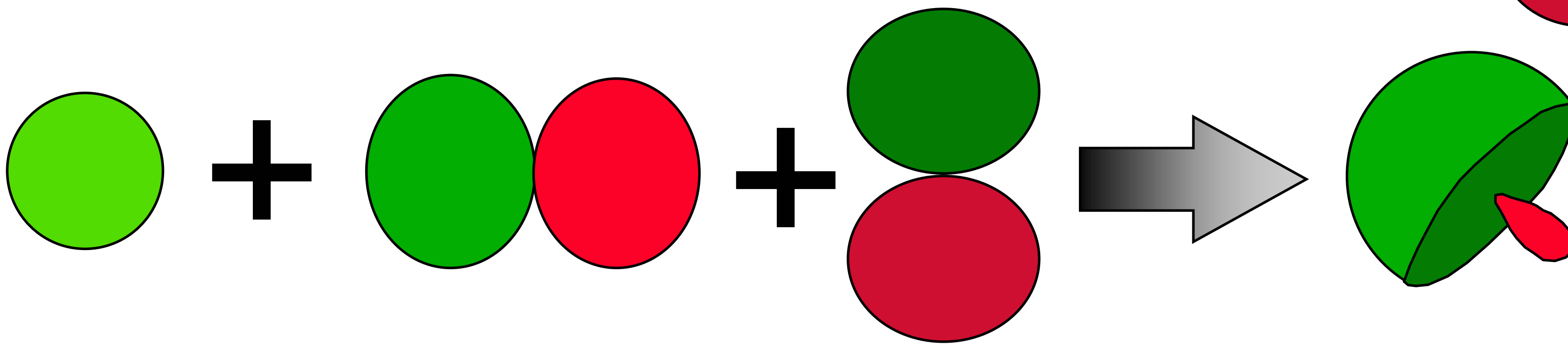
B: $1s^2\ 2s^2\ 2p^1$

3) Draw energy diagram for the atom and decouple paired electrons:

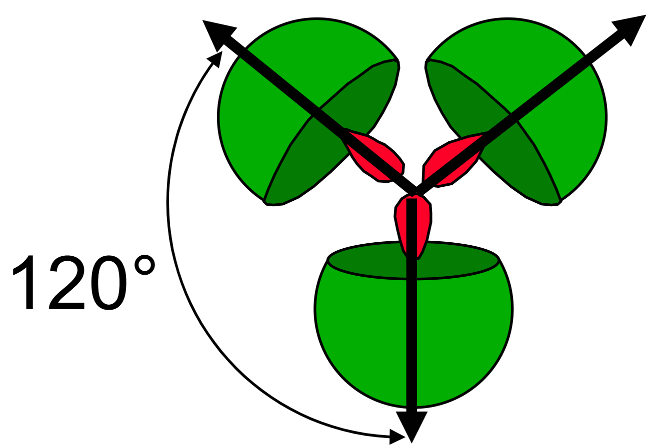


4) <u>Take linear combinations of the atomic orbitals participating in the bond to make hybrid orbitals:</u>

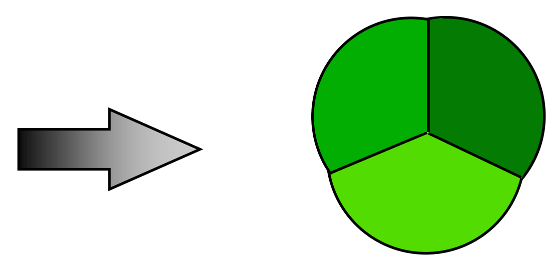




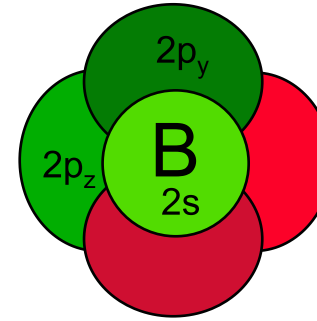
We know that if we start with three orbitals,we must finish with three orbitals. Thus, they will be 120° apart:

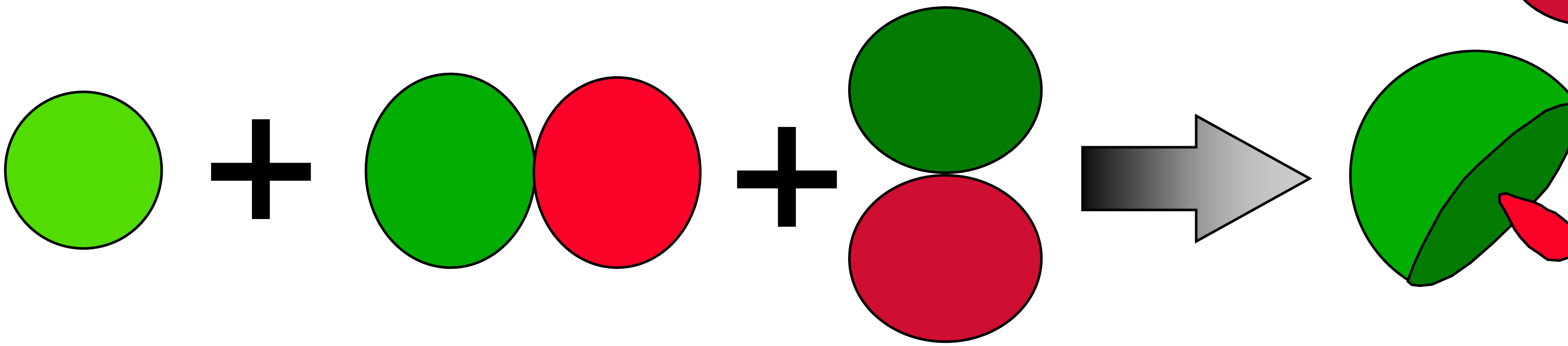


The orbitals are centered at the node between the green and red lobes, so the orbitals overlap.

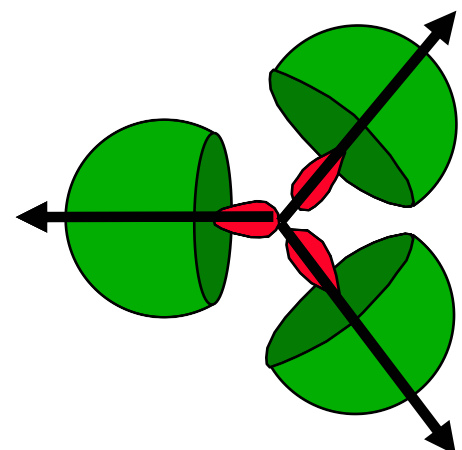


4) Take linear combinations of the atomic orbitals participating in the bond to make hybrid orbitals:

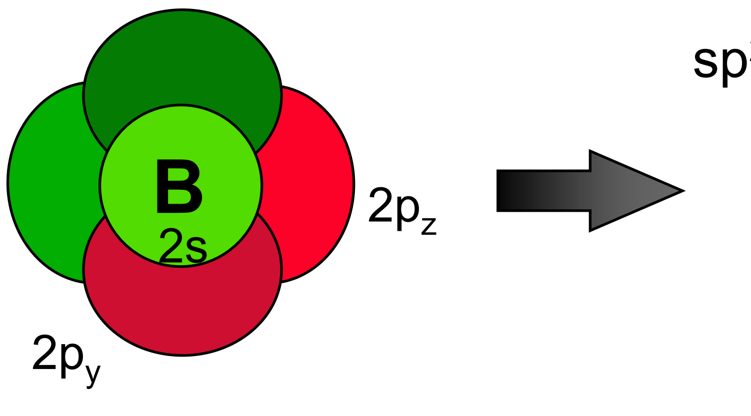




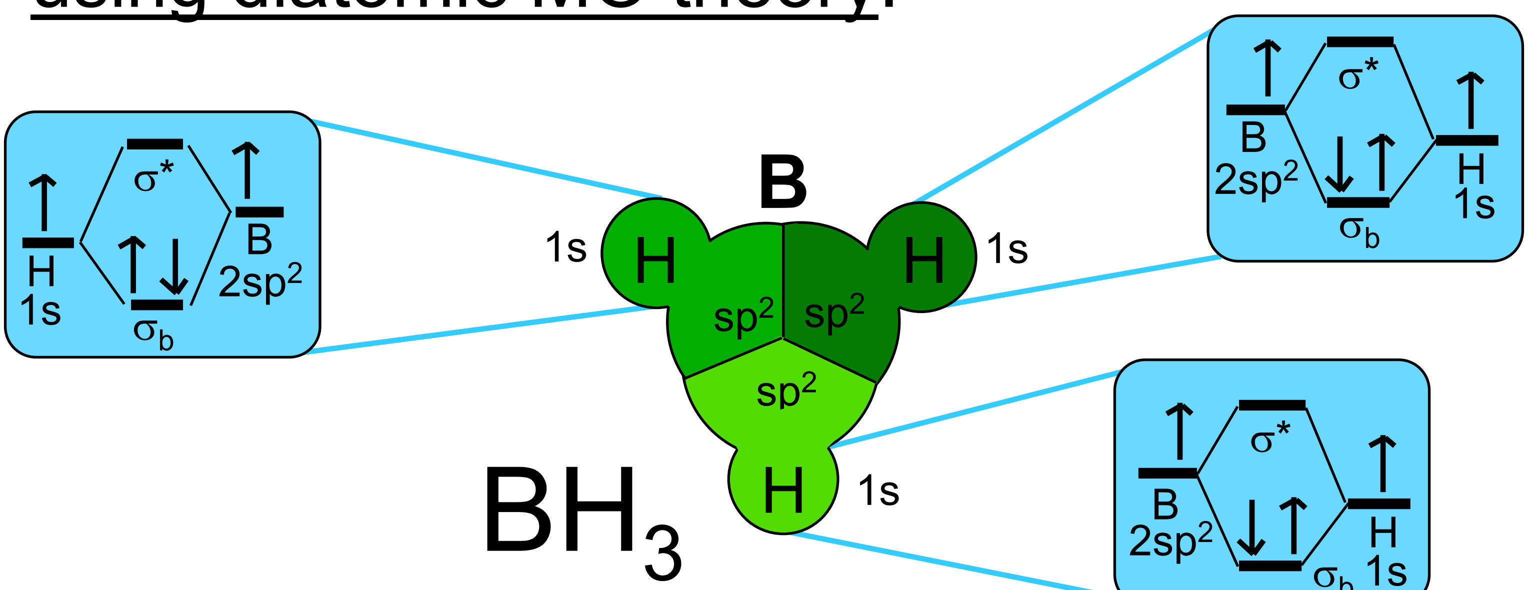
1/√3	**+**	**2/√6**		
1/√3	**-**	**1/√6**	**+**	**1/√2**
1/√3	**-**	**1/√6**	**-**	**1/√2**



4′) Take linear combinations of the atomic orbitals participating in the bond to make hybrid orbitals:



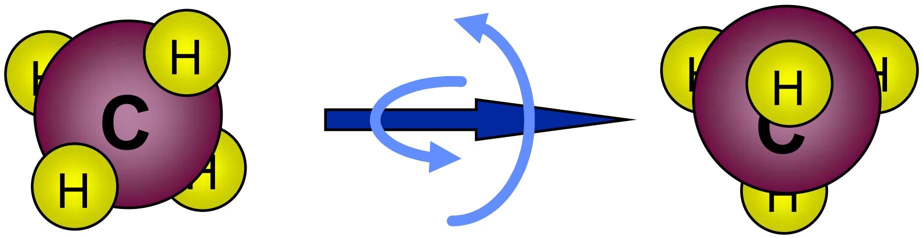
5) Combine hybrid orbitals with other atoms' orbitals using diatomic MO theory:

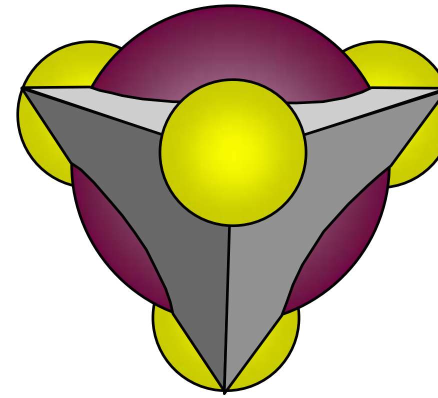


Make CH_4:

We know:

- The geometry, from VSEPR:



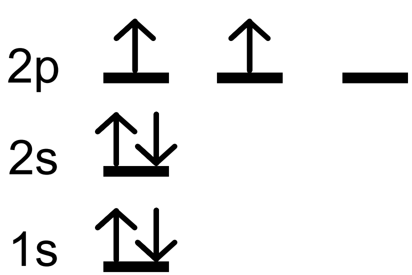


Bond angle: 109.5°

Tetrahedral

- The electron configurations:

C: $1s^2\ 2s^2\ 2p^2$

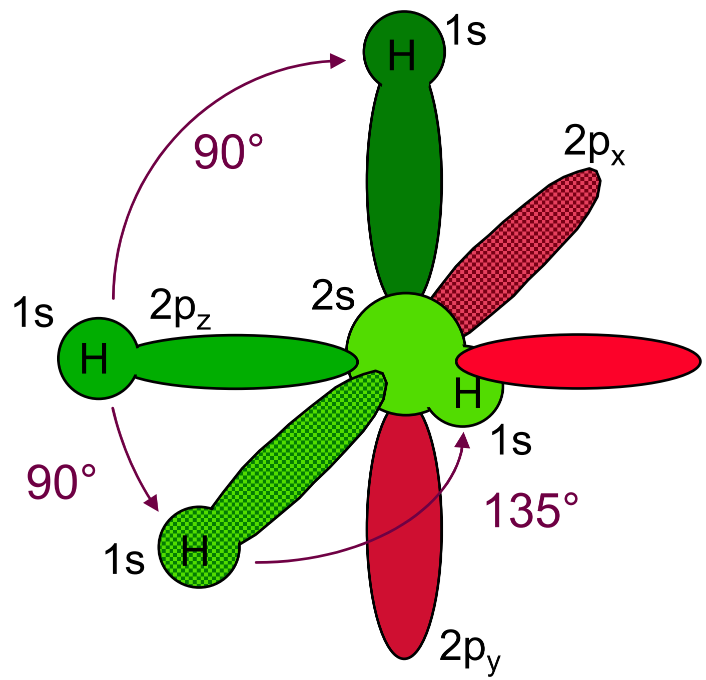


H: $1s^1$

Make CH_4:

What does this look like in terms of orbitals?

Possibilities:



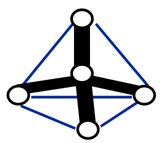
WRONG: This shape doesn't match the one predicted by VSEPR.

Use what we learned about hybrids:

CH_4

1) Assign Geometry Using VSEPR:

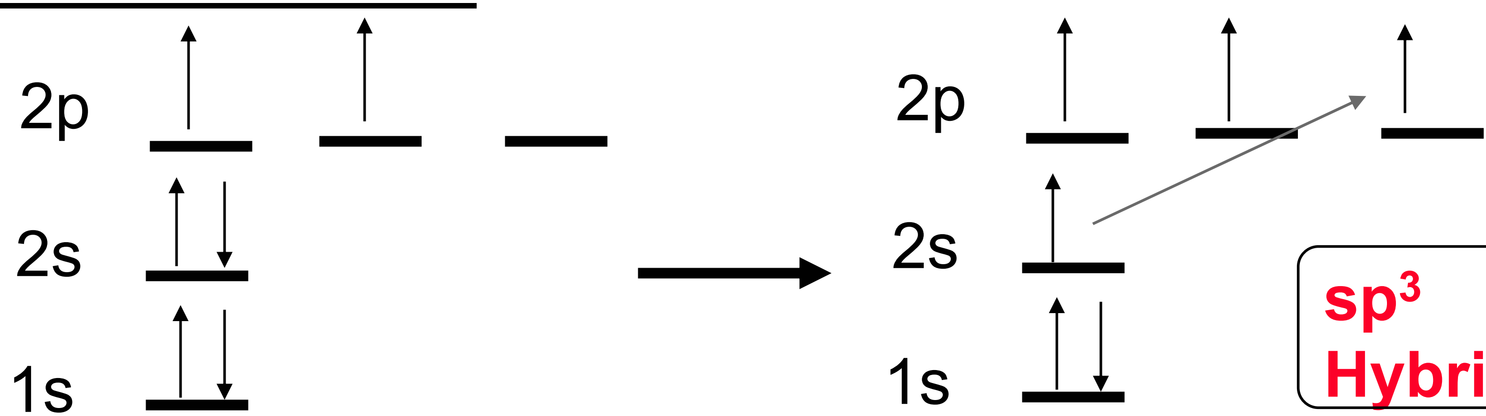
CH_4 SN = 4 Geometry: Tetraheadral



2) Write electron configuration of atom to be hybridized:

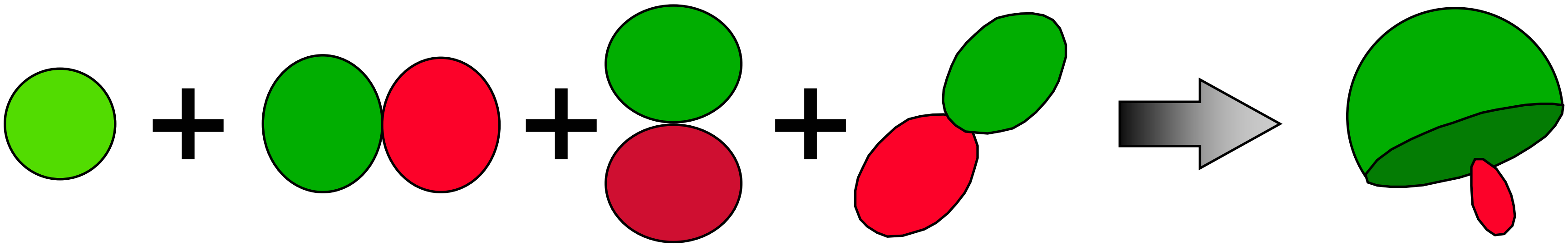
C: $1s^2\ 2s^2\ 2p^2$

3) Draw energy diagram for atom and decouple paired electrons:

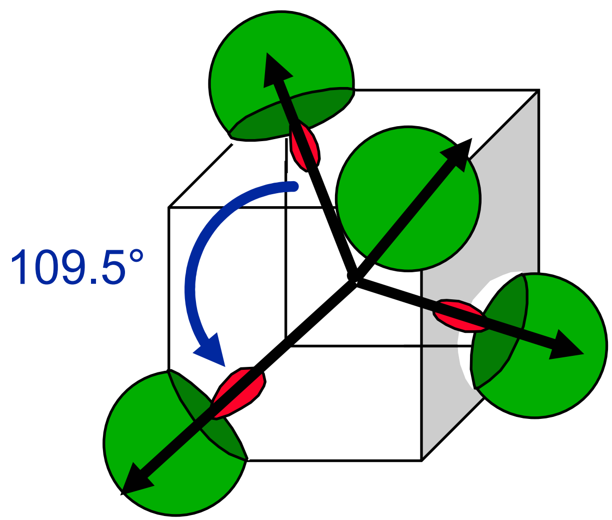


sp^3 Hybrids

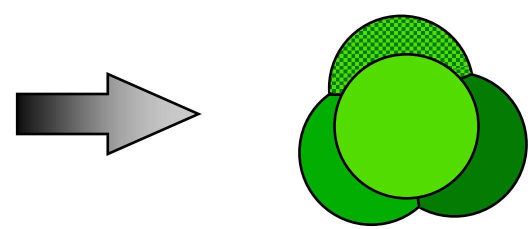
4) Take linear combinations of participating atomic orbitals to make hybrid orbitals:



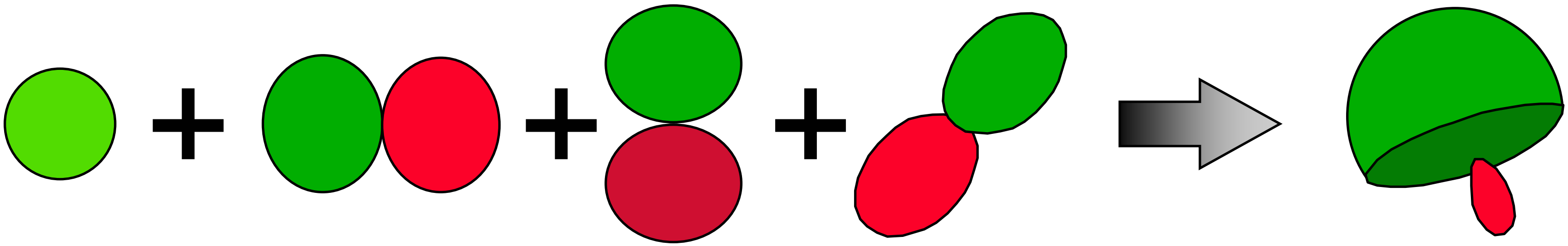
We know that if we start with four orbitals, we must finish with four orbitals. Thus, they will be 109.5° apart:



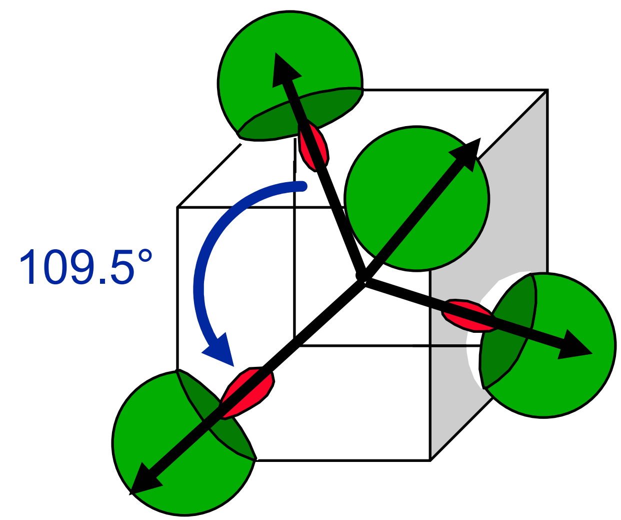
The orbitals are centered at the node between the green and red lobes, so the orbitals overlap.



4) <u>Take linear combinations of participating atomic orbitals to make hybrid orbitals:</u>



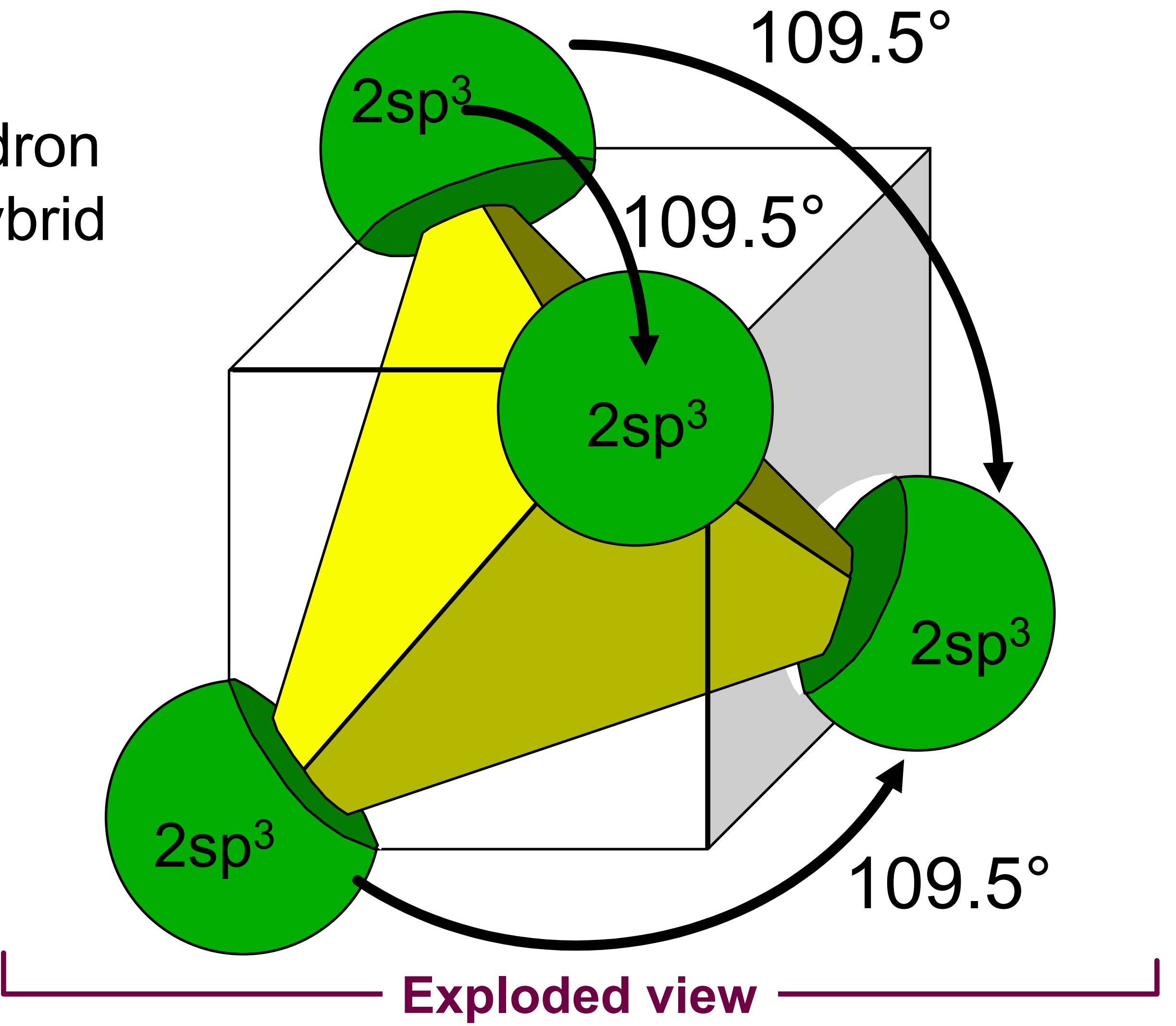
1/2	+	1/2	+	1/2	+	1/2
1/2	-	1/2	-	1/2	+	1/2
1/2	-	1/2	+	1/2	-	1/2
1/2	+	1/2	-	1/2	-	1/2



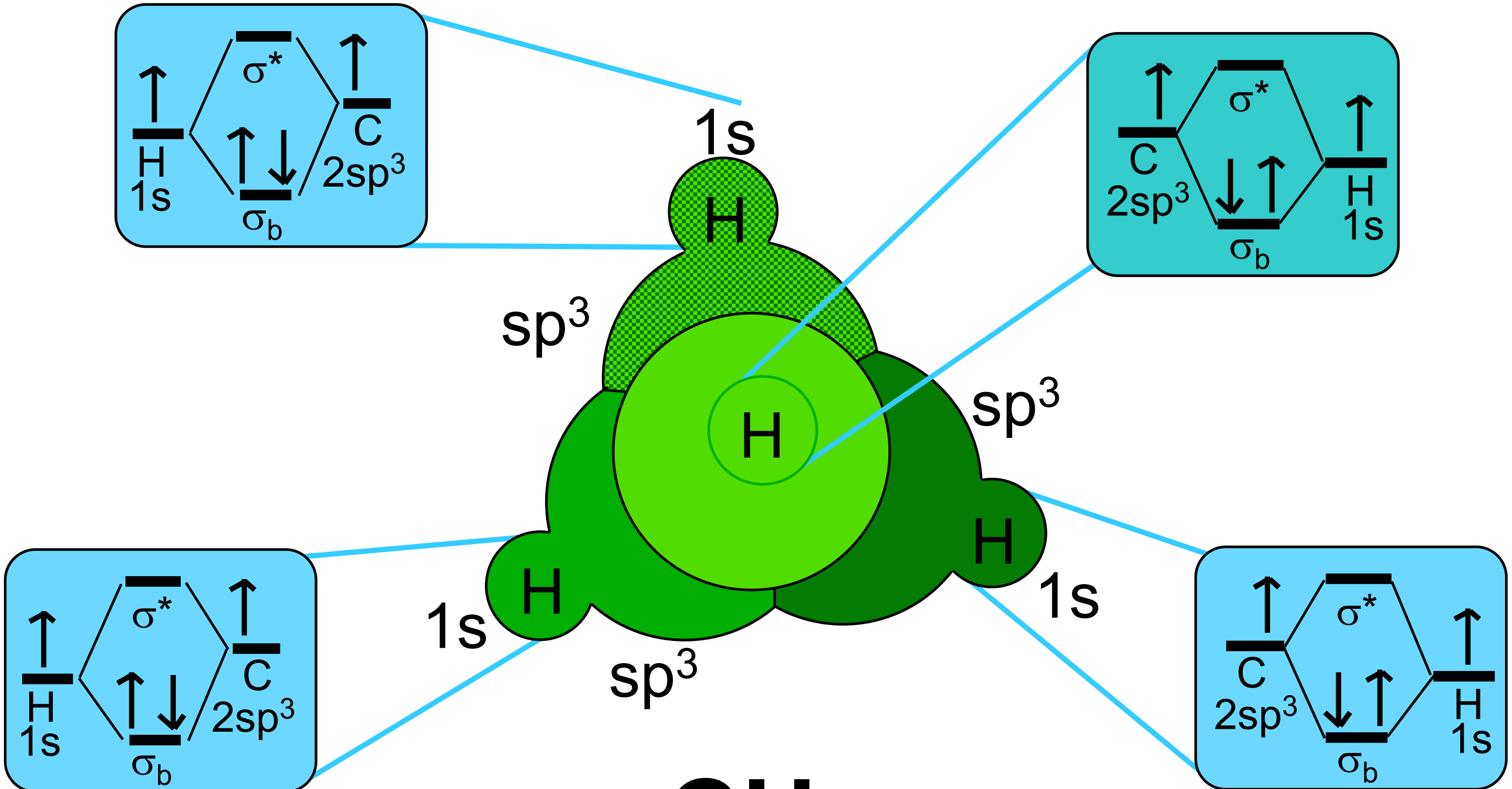
4) Take linear combinations of participating atomic orbitals to make hybrid orbitals:

Notice the tetrahedron formed by the sp^3 hybrid orbitals.

This is the shape predicted for CH_4 by VSEPR.



5) Combine hybrid orbitals with other atoms' orbitals using diatomic MO theory:



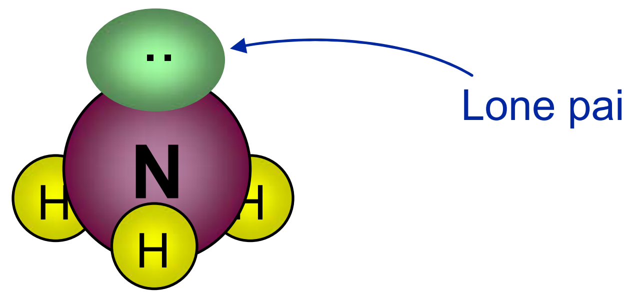
CH_4

- All the angles are correct.
- All the orbitals have the same energy.

Make NH_3:

We know:

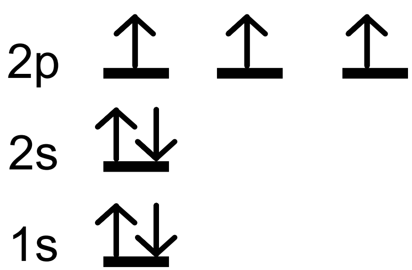
- It has one lone pair.
- The geometry, from VSEPR:



Bond angle: <109.5°

- The electron configurations:

N: $1s^2\ 2s^2\ 2p^3$

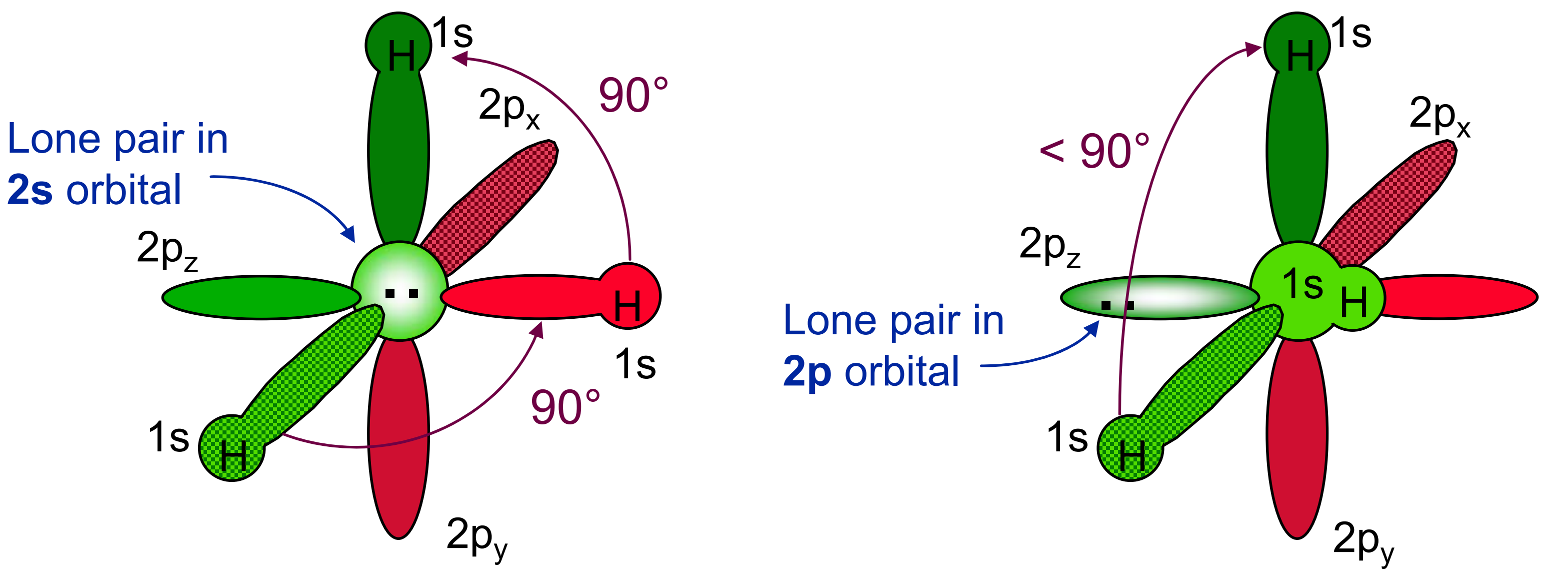


H: $1s^1$

Make NH_3:

What does this look like in terms of orbitals?

Possibilities:

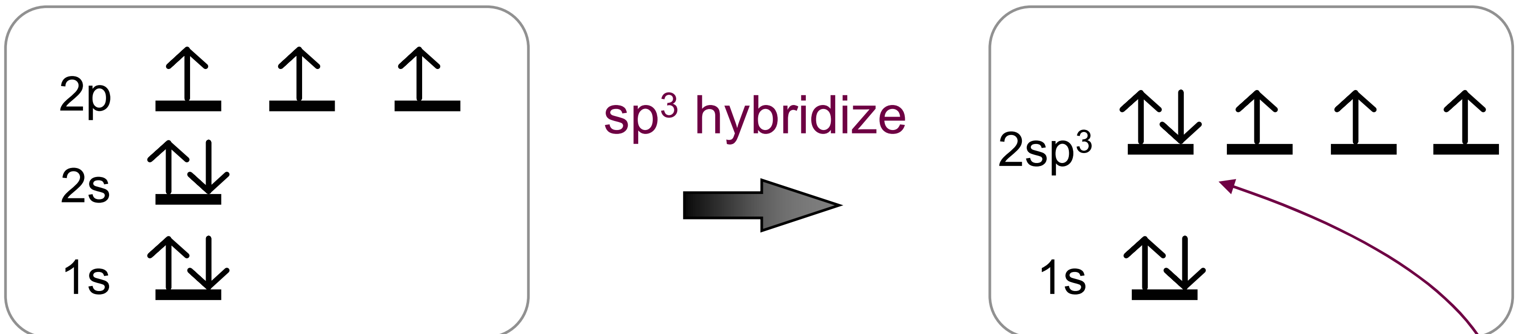


WRONG: The shapes don't match those predicted by VSEPR.

Make NH_3:

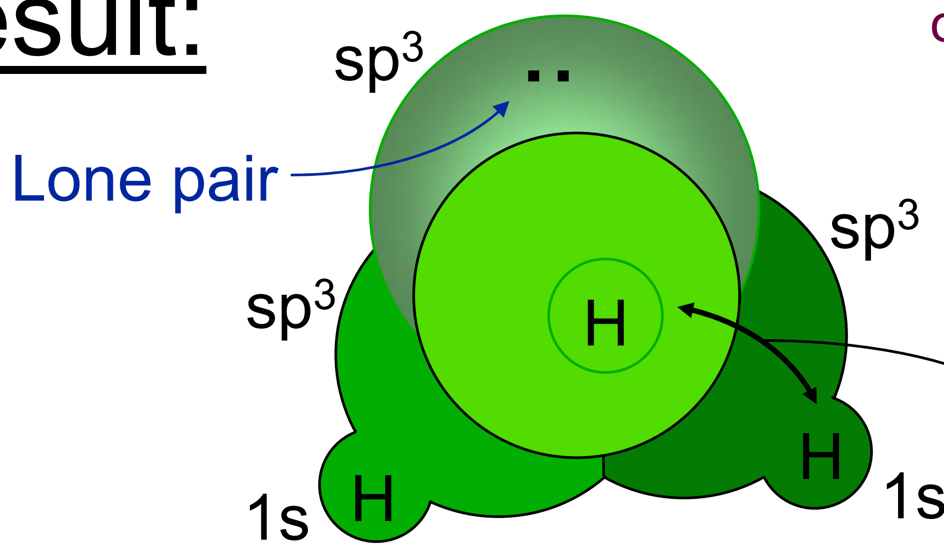
NH_3 has a steric number of 4.

This suggests we should use sp^3 hybridization



Notice one of the sp^3 orbitals has the lone pair

Result:

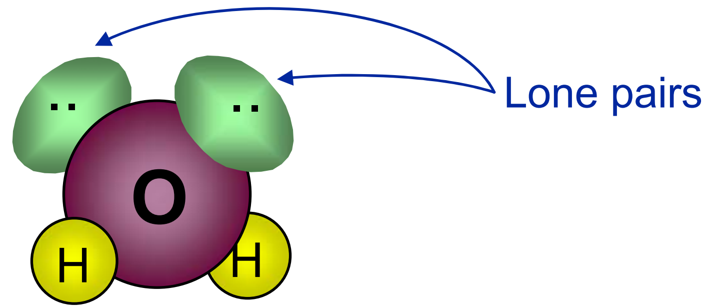


Slightly less than 109.5° because lone pairs are **fat**!

Make H_2O:

We know:

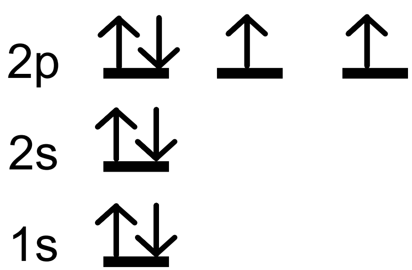
- The molecule has two lone pairs.
- The geometry, from VSEPR:



Bond angle: <109.5° (104.5°)

- The electron configurations:

O: $1s^2\ 2s^2\ 2p^4$

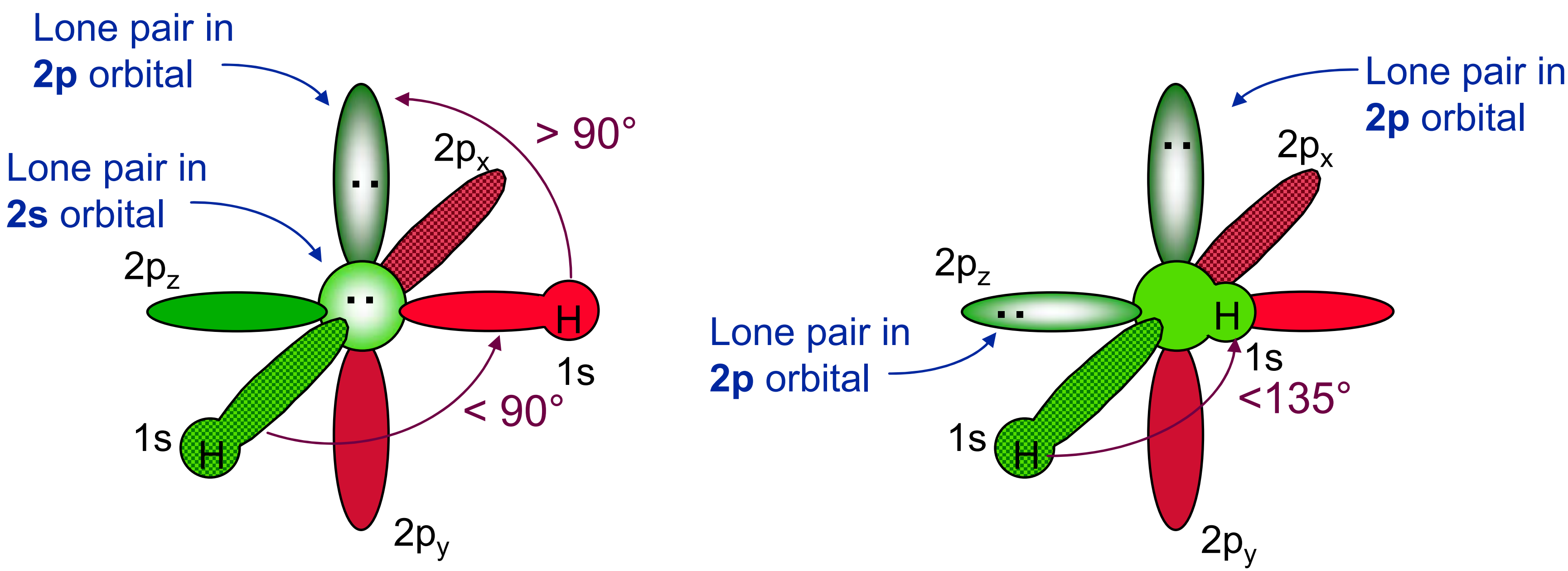


H: $1s^1$

Make H_2O:

What does this look like in terms of orbitals?

Possibilities:

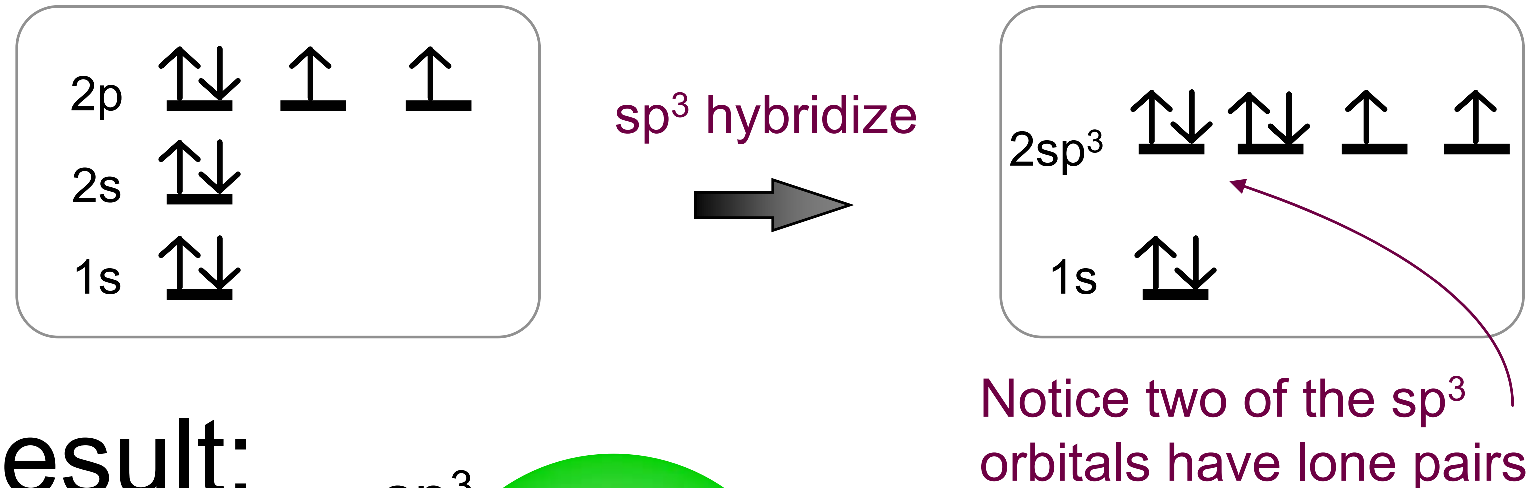


WRONG: These shapes don't match those predicted by VSEPR.

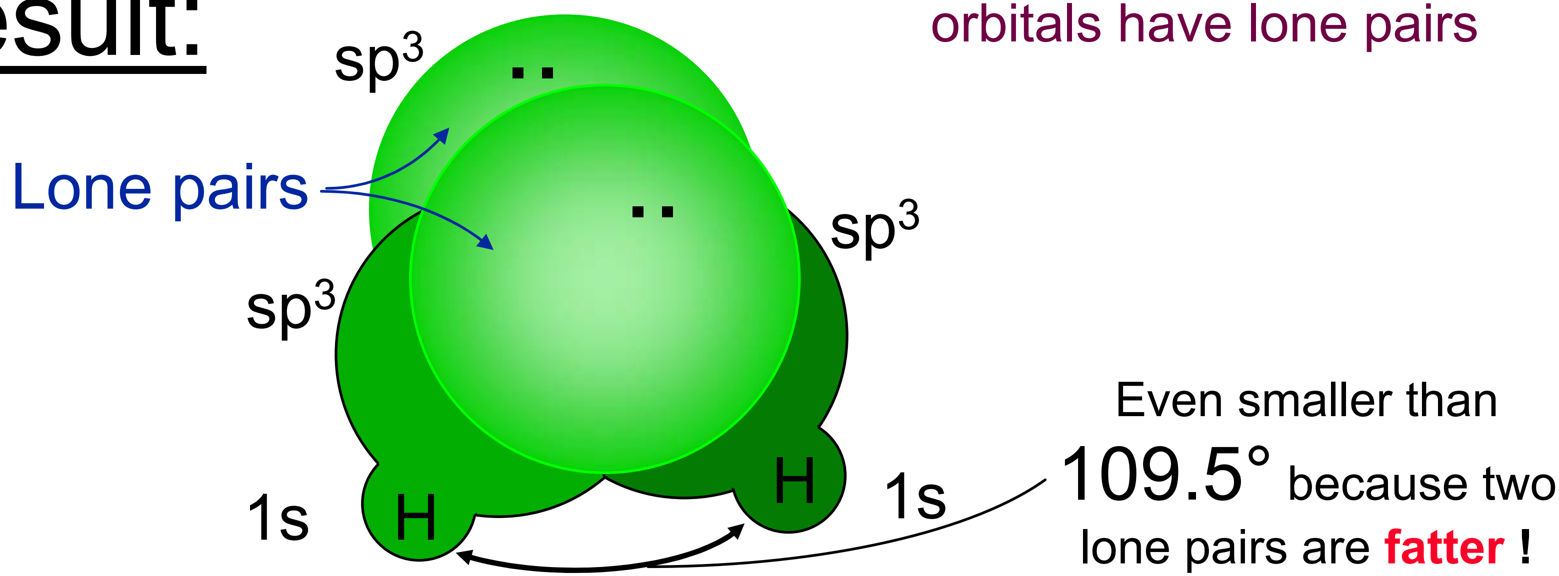
Make H_2O:

H_2O has a steric number of 4.

This suggests we should use sp^3 hybridization



Result:



End

of

Hybridization

Part 1

Reading: Gray: (4-1), (4-2), and (4-4)
OGN: (16.2)