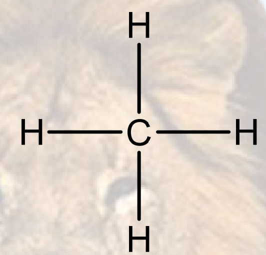
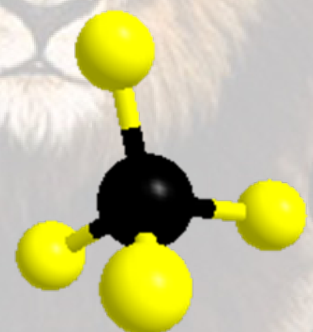
# Hybrid Orbitals

# The Methane Problem

- The Lewis structure for methane ($CH_4$) is:

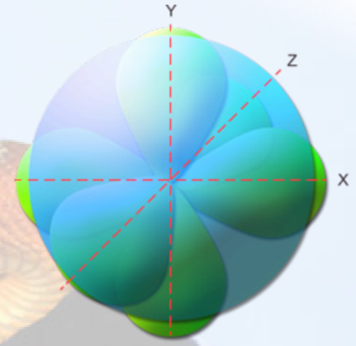



- Based on the VSEPR model, the shape is tetrahedral.

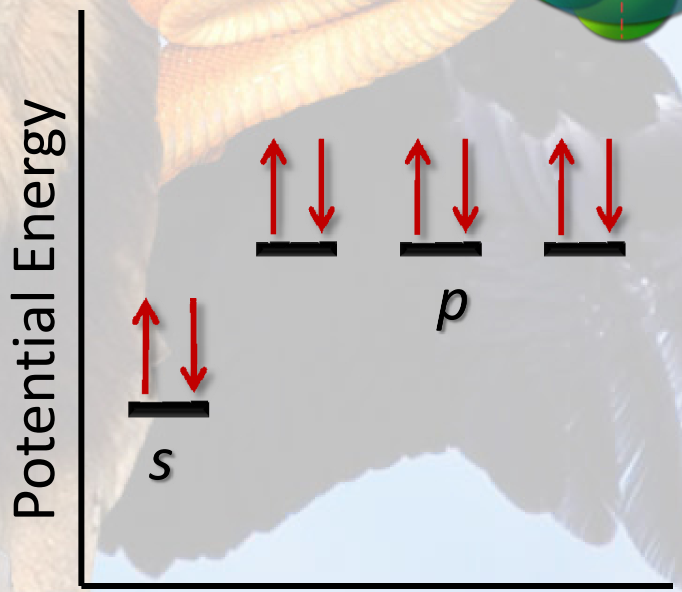


- The electron dot diagram for carbon is $\underset{\cdot}{\ddot{\mathrm{C}}}\cdot$
- How do you get four bonds at 109° from two unpaired electrons in *p* orbitals at 90°?

# The Atomic Orbital Conundrum



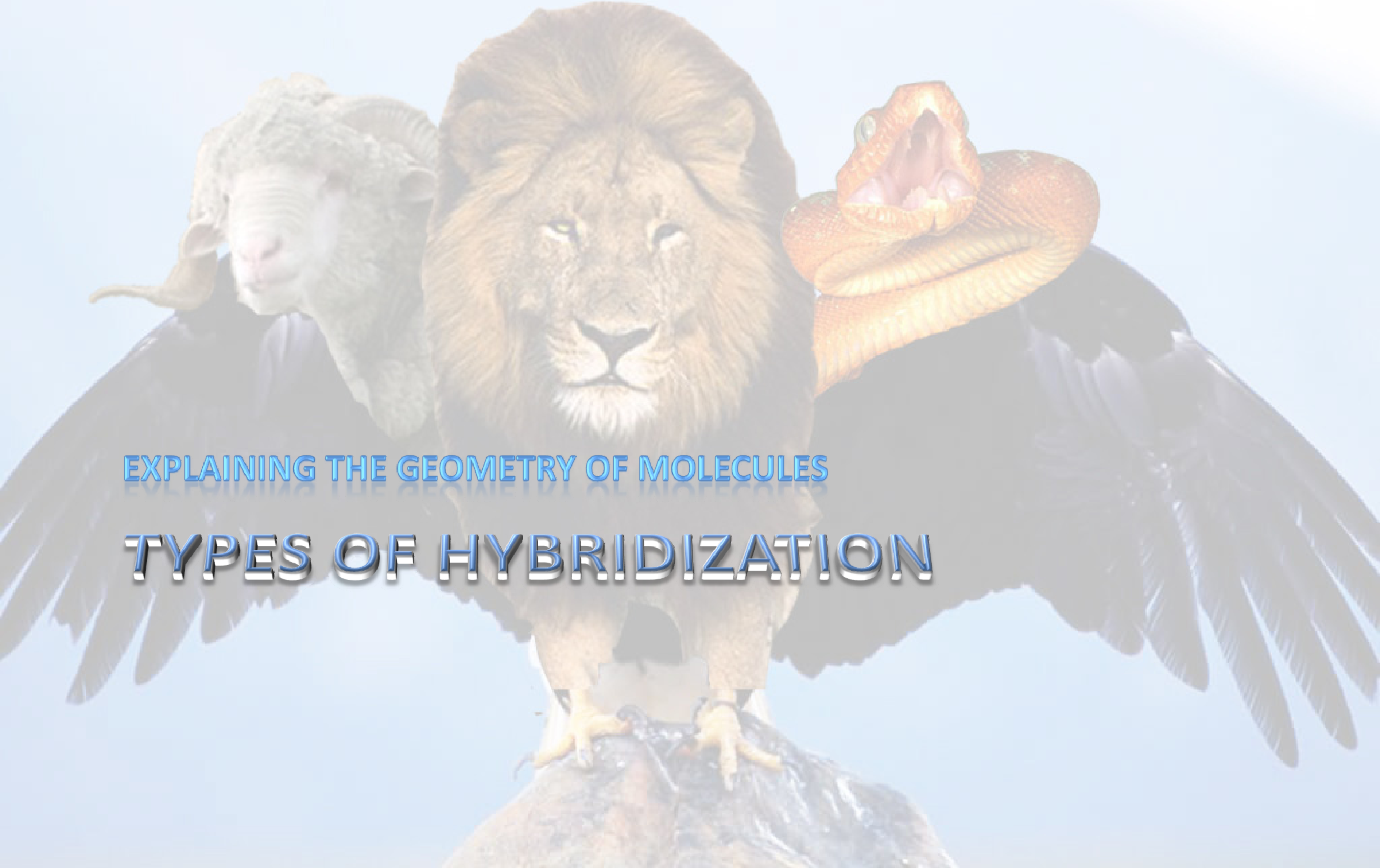

- The valence shell for the main group elements consists of one *s* orbital and 3 *p* orbitals at right angles to each other.
- The *s* sublevel is lower energy than the *p* sub-level.
  - The orbital in the *s* sublevel fills first.
  - The 3 orbitals in the *p* sublevel each get one electron before pairing. (Hund's rule)
- This accounts for the appearance of carbon, $\ddot{\mathrm{C}}\cdot$,




. . . but it does not account for the geometry of carbon compounds.

# Hybridization

- When electrons are shared, they are at lowest energy between the nuclei that are sharing them.
- Their most probable locations are no longer in the atomic orbitals where they were, but rather in new, molecular orbitals.
    - A good description of these orbitals comes from hybridization theory.
- **Hybridization** = mixing of atomic orbitals to form new orbitals

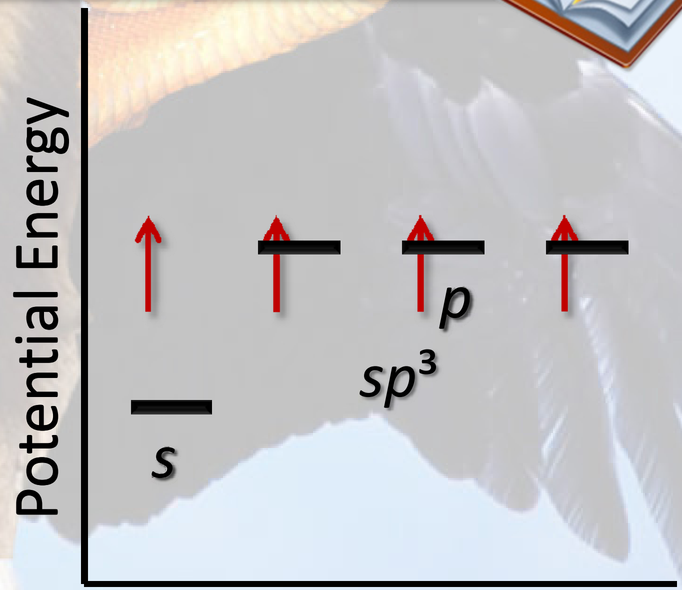


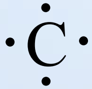
## EXPLAINING THE GEOMETRY OF MOLECULES

# TYPES OF HYBRIDIZATION

# $sp^3$ Hybridization

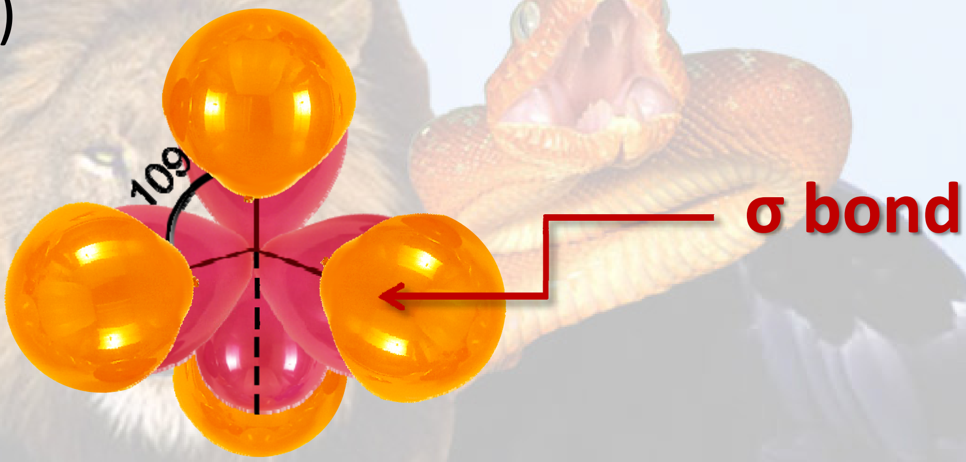
- *$sp^3$* hybrid orbitals are formed by combining one *s* orbital with three *p* orbitals to form four equal energy orbitals.
- Since the four orbitals are equal energy, one electron goes into each before pairing.
- This gives carbon four unpaired electrons.



# More on $sp^3$ Hybridization

- The four *sp*³ hybrid orbitals are at 109°. (Imagine tying four balloons together.)



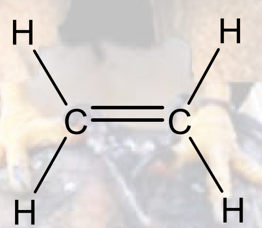

- When carbon bonds with four hydrogens to form methane, the *s* orbitals overlap the four *sp*³ orbitals to form sigma bonds (σ bonds).
  - sigma bond – bond formed by sharing a pair of electrons in an area centered on a line between two atoms.
- Whenever an atom is surrounded by four effective electron pairs, *sp*³ hybrid orbitals are required.

WRITE DOWN

# $sp^2$ Hybridization

WRITE DOWN

- Whenever an atom is surrounded by three effective electron pairs to form a trigonal planar molecule, a set of $sp^2$ hybrid orbitals is required.
- Combination of one *s* orbital and two *p* orbitals to form an $sp^2$ hybrid gives the appropriate 120° angle.
  - In forming the $sp^2$ orbital, one *p* orbital is not used, and is oriented perpendicular to the plane of the $sp^2$ orbitals.
- Example: Ethene ($C_2H_4$), has three effective pairs of electrons around each carbon (the double bond acts as one effective pair)



# Bonding by sp² Hybridization

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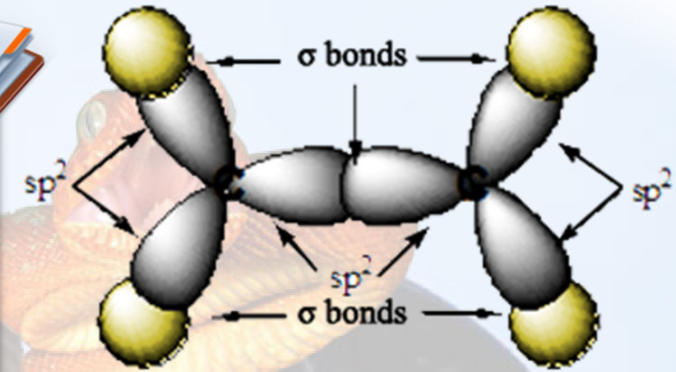
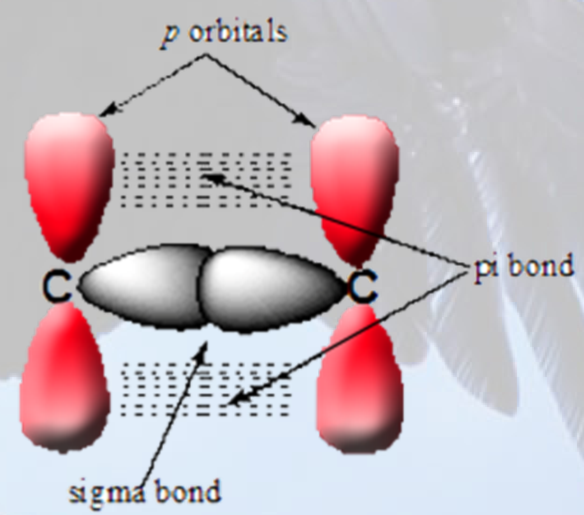
- Each of the three *sp*² orbitals forms bonds by sharing a pair of electrons in an area centered on a line between the two atoms.
  - These are called sigma (σ) bonds.
- The double bond is formed in the space above and below the σ bond by the *p* orbital perpendicular to the *sp*² orbitals.
  - This is called a pi (π) bond.

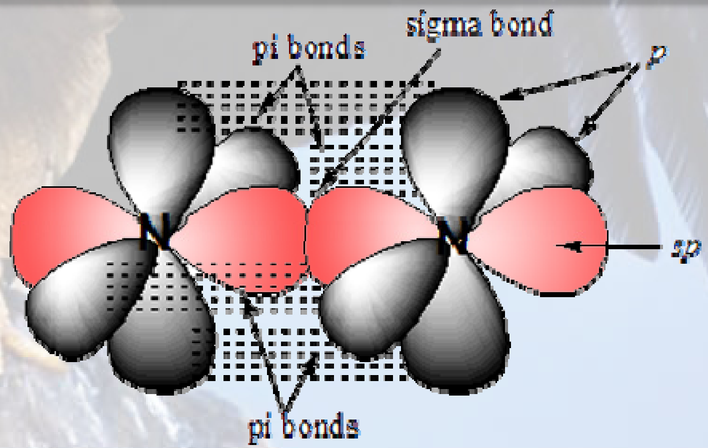


# sp Hybridization

WRITE DOWN

- *sp* hybridization enables two effective pairs of electrons to bond at 180°.
  - One *s* and one *p* are hybridized to form two *sp* hybrid orbitals at a 180° angle.
  - Two *p* orbitals remain.
- The hybrid orbitals form sigma bonds and the *p* orbitals form pi bonds.
- Examples
  - $CO_2$
  - $C_2H_2$
  - $N_2$



# $dsp^3$ Hybridization

WRITE DOWN

- *dsp*$^3$ hybridization enables a trigonal bipyrimidal arrangement for five pairs of electrons surrounding a central atom.
- Forms from one *d* orbital, one *s* orbital, and three *p* orbitals.
- Examples
  - $PCl_5$
  - $I_3^-$

# $d^2sp^3$ Hybridization


- $d^2sp^3$ hybridization enables an octahedral arrangement for six pairs of electrons surrounding a central atom.
  - Forms from two *d* orbitals, one *s* orbital, and three *p* orbitals.
- Examples
  - $SF_6$
  - $XeF_4$ (Xe has two lone pairs)