

## PHYS 3320 $sp^n$ hybrid orbitals

$$ns^2 np^2 \rightarrow ns^1 np^3$$

remaining s electron can hybridize with one or more p orbitals (px, py, pz)

### I) $sp^1$ hybrid orbitals ( $180^\circ$ )

$$\phi_1 = (\phi_s + \phi_{px})/2^{1/2}$$



$$\phi_2 = (\phi_s - \phi_{px})/2^{1/2}$$



$p_y$

$p_z$

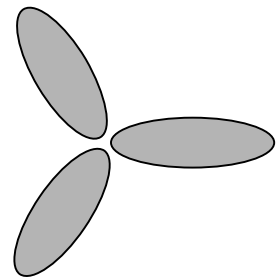
### II) $sp^2$ hybrid orbitals ( $120^\circ$ )

$$\phi_1 = (1/3^{1/2}) [ \phi_s + 2^{1/2} \phi_{px} ]$$

$$\phi_2 = (1/3^{1/2}) [ \phi_s - (1/2)^{1/2} \phi_{px} + (3/2)^{1/2} \phi_{py} ]$$

$$\phi_3 = (1/3^{1/2}) [ \phi_s - (1/2)^{1/2} \phi_{px} - (3/2)^{1/2} \phi_{py} ]$$

$p_z$



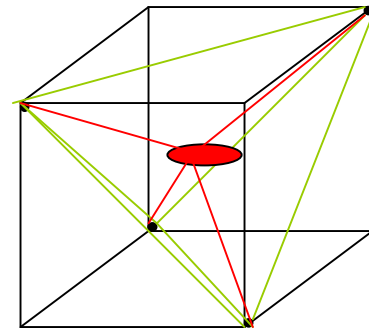
### III) $sp^3$ hybrid orbitals ( $109.5^\circ$ )

$$\phi_1 = (1/2) [ \phi_s + \phi_{px} + \phi_{py} + \phi_{pz} ]$$

$$\phi_2 = (1/2) [ \phi_s + \phi_{px} - \phi_{py} - \phi_{pz} ]$$

$$\phi_3 = (1/2) [ \phi_s - \phi_{px} + \phi_{py} - \phi_{pz} ]$$

$$\phi_4 = (1/2) [ \phi_s - \phi_{px} - \phi_{py} + \phi_{pz} ]$$



Note that all orbitals are normalized and are orthogonal, e.g.

Integral  $(\phi_1 \phi_1) dx dy dz = 1$  and Integral  $(\phi_j \phi_k) dx dy dz = 0$  if  $j \neq k$  !