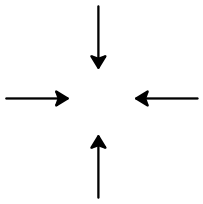
XeF_4 SALCs
Sigma Bonding



$$\Gamma_\sigma = A_{1g} + B_{1g} + E_u$$

✔ Use the C_4 character table to read off the projections for the SALCs.

C_4	E	C_4	C_2	C_4^3
A	1	1	1	1
B	1	-1	1	-1
E^a	1	i	-1	$-i$
E^b	1	$-i$	-1	i

✔ Projections:

$$P(A) \propto (\phi_1 + \phi_2 + \phi_3 + \phi_4)$$
$$P(B) \propto (\phi_1 - \phi_2 + \phi_3 - \phi_4)$$
$$P(E^a) \propto (\phi_1 + i\phi_2 - \phi_3 - i\phi_4)$$
$$P(E^b) \propto (\phi_1 - i\phi_2 - \phi_3 + i\phi_4)$$

✔ Obtaining Real Functions:

$$P(E^a) + P(E^b) \propto (\phi_1 - \phi_3)$$
$$P(E^a) - P(E^b) \propto (\phi_2 - \phi_4)$$

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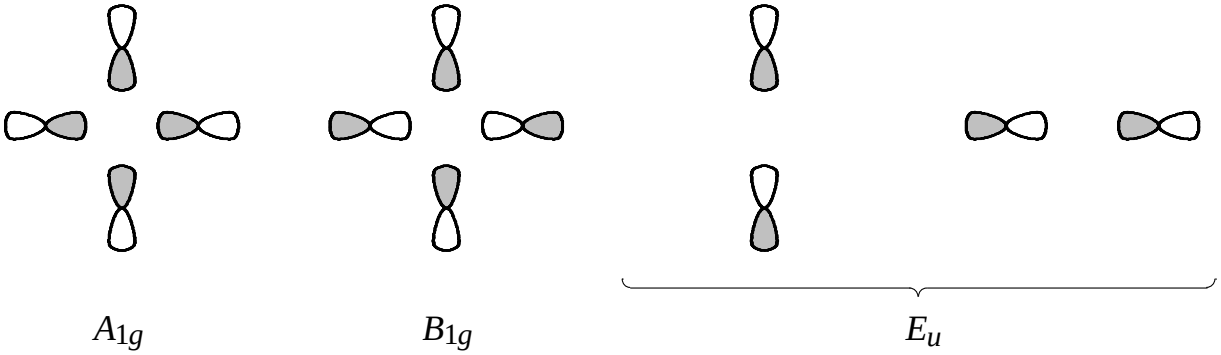
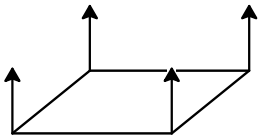
☞ Normalized SALCs:

$$\Phi(A) = \tfrac{1}{2}(\phi_1 + \phi_2 + \phi_3 + \phi_4)$$
$$\Phi(B) = \tfrac{1}{2}(\phi_1 - \phi_2 + \phi_3 - \phi_4)$$
$$\Phi(E^{\alpha}) = 1/\sqrt{2}(\phi_1 - \phi_3)$$
$$\Phi(E^{\beta}) = 1/\sqrt{2}(\phi_2 - \phi_4)$$



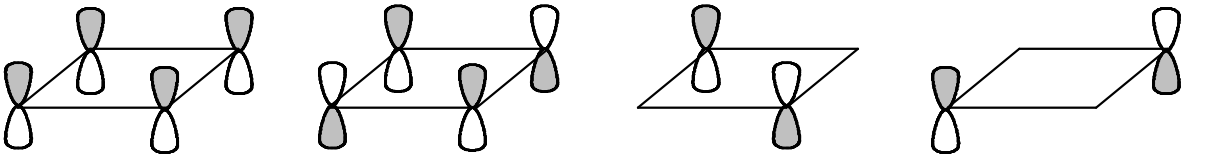
A_{1g} B_{1g} E_u

XeF_4 SALCs
Pi($\perp$) Bonding



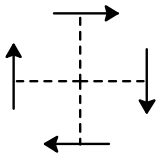
$$\Gamma_{\perp} = E_g + A_{2u} + B_{2u}$$

✔ In C_4 these species are $A + B + E$, so the mathematical forms of these SALCs are the same as the sigma SALCs.



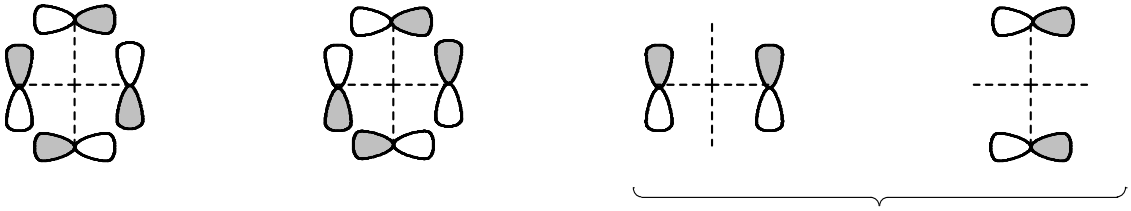
A_{2u} B_{2u} E_g

XeF_4 SALCs Revisited
Pi(∥) Bonding



$$\Gamma_{\parallel} = A_{2g} + B_{2g} + E_u$$

✔ Also $A + B + E$ in C_4, so the forms of the SALCs are once again the same.



A_{2g} B_{2g} E_u