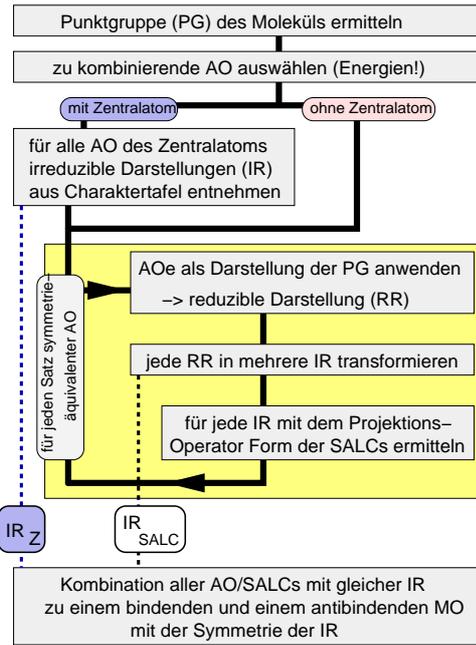


2. LCAO-Ansatz: Der Festkörper als 'Riesenmolekül' (Forts.)

2.1.2. Molekülorbitale (Forts.)

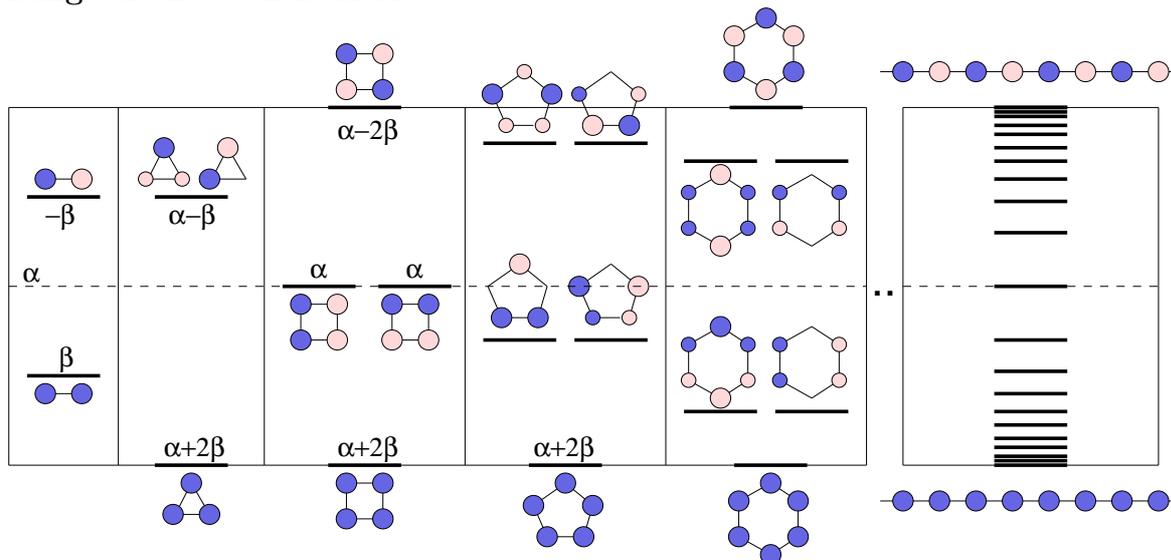
Charaktertafel der Punktgruppe D_{4h}

	E	C_4	C_2	C_2'	C_2''	i	S_4	σ_h	σ_v	σ_d		
A_{1g}	1	1	1	1	1	1	1	1	1	1	R_z	$x^2 + y^2, z^2$
A_{2g}	1	1	1	-1	-1	1	1	1	-1	-1		$x^2 - y^2$
B_{1g}	1	-1	1	1	-1	1	-1	1	1	-1	(R_x, R_y)	xy
B_{2g}	1	-1	1	-1	1	1	-1	1	-1	1		(xz, yz)
E_g	2	0	-2	0	0	2	0	-2	0	0		
A_{1u}	1	1	1	1	1	-1	-1	-1	-1	-1		
A_{2u}	1	1	1	-1	-1	-1	-1	-1	1	1	z	
B_{1u}	1	-1	1	1	-1	-1	1	-1	-1	1		
B_{2u}	1	-1	1	-1	1	-1	1	-1	1	-1		
E_u	2	0	-2	0	0	-2	0	2	0	0		(x, y)
4 s	4	0	0	2	0	0	0	4	2	0		$a_{1g} + b_{1g} + e_u$
4 p _x	4	0	0	2	0	0	0	4	2	0		$a_{1g} + b_{1g} + e_u$



2.2. 1-dimensional unendlicher Fall

Ringe als LC von 1s-H-AO



1s-H-Atomkette: LCAO, DOS, Bandstruktur, COOP

