






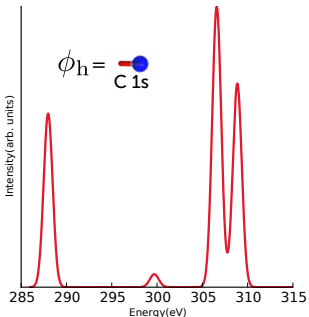


	ϕ_i		Ω_i
5A ₁		. . .	0.008
1B ₂		. . .	0.000
1B ₁		. . .	0.000
4A ₁		. . .	0.008
3A ₁		. . .	0.007
2A ₁		. . .	0.976
1A ₁		. . .	0.000

a) Evaluate Subspace occupation of each occupied orbital for C 1s subspace



b) Hole orbital is chosen as the C1s orbital. C K-Edge is calculated directly.