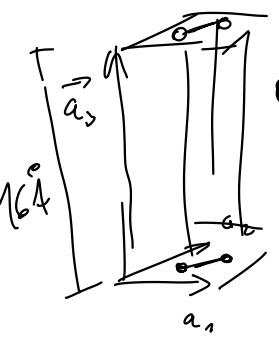
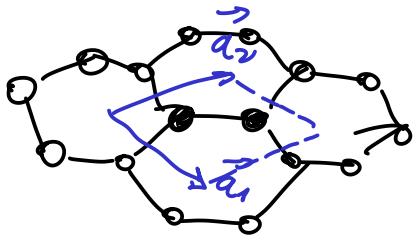
Graphene – single sheet of graphite

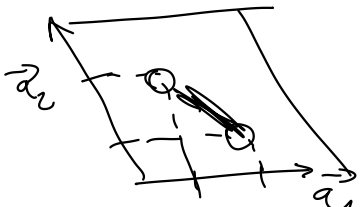




vdW ↕ ~3.3 Å

c

(a, b)



ibrav = 4

cell dm (1) ---- $|\vec{a}_1| = |\vec{a}_2| = 4.627$ Å bohr = 2.46 Å

cell dm (3) --- 4.879

4.879 × 4.647 = ... 16 Å

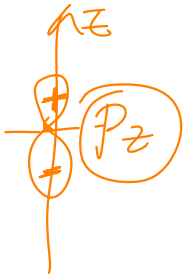
principal axis of rotation
6-fold
↓
6 → 2-fold axes perpendicular
↓
horizontal mirror plane

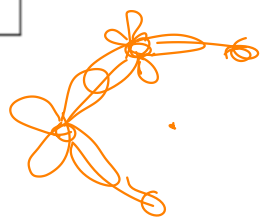
D_{6h}

24 = 1 2 2 1

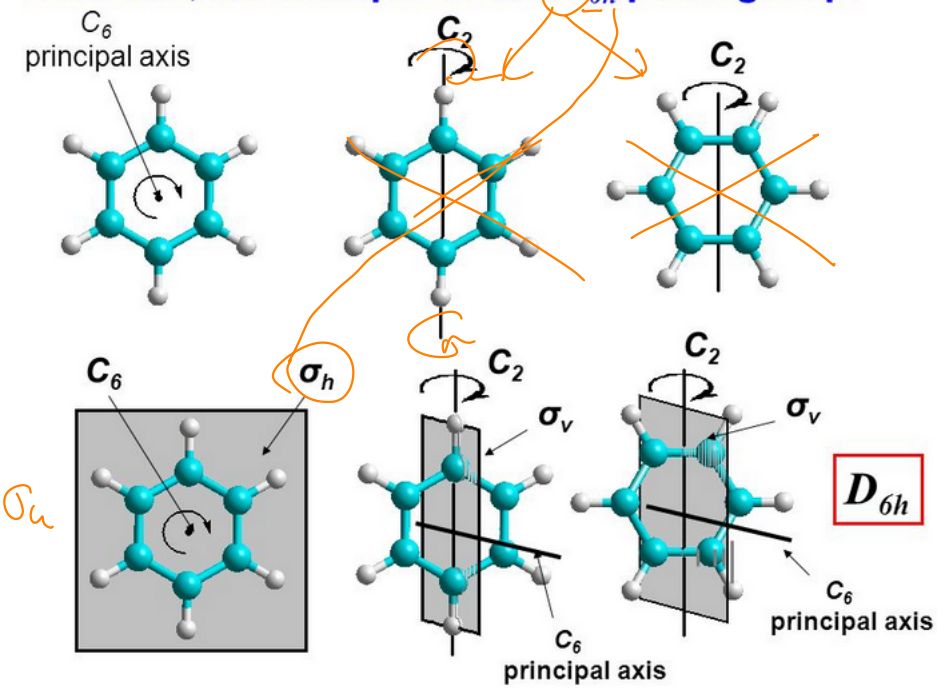
Character table for D_{6h} point group

	E	$2C_6$	$2C_3$	C_2	$3C'_2$	$3C''_2$	i	$2S_3$	$2S_6$	σ_h	$3\sigma_d$	$3\sigma_v$	Linear, rotations	Quadratic
A_{1g}	1	1	1	1	1	1	1	1	1	1	1	1		x^2+y^2, z^2
A_{2g}	1	1	1	1	-1	-1	1	1	1	1	-1	-1	R_z	
B_{1g}	1	-1	1	-1	1	-1	1	-1	1	-1	1	-1		
B_{2g}	1	-1	1	-1	-1	1	1	-1	1	-1	-1	1		
E_{1g}	2	1	-1	-2	0	0	2	1	-1	-2	0	0	(R_x, R_y)	(xz, yz)
E_{2g}	2	-1	-1	2	0	0	2	-1	-1	2	0	0		(x^2-y^2, xy)
A_{1u}	1	1	1	1	1	1	-1	-1	-1	-1	-1	-1		
A_{2u}	1	1	1	1	-1	-1	-1	-1	-1	-1	1	1	z	
B_{1u}	1	-1	1	-1	1	-1	-1	1	-1	1	-1	1		
B_{2u}	1	-1	1	-1	-1	1	-1	1	-1	1	1	-1		
E_{1u}	2	1	-1	-2	0	0	-2	-1	1	2	0	0	(x, y)	
E_{2u}	2	-1	-1	2	0	0	-2	1	1	-2	0	0		



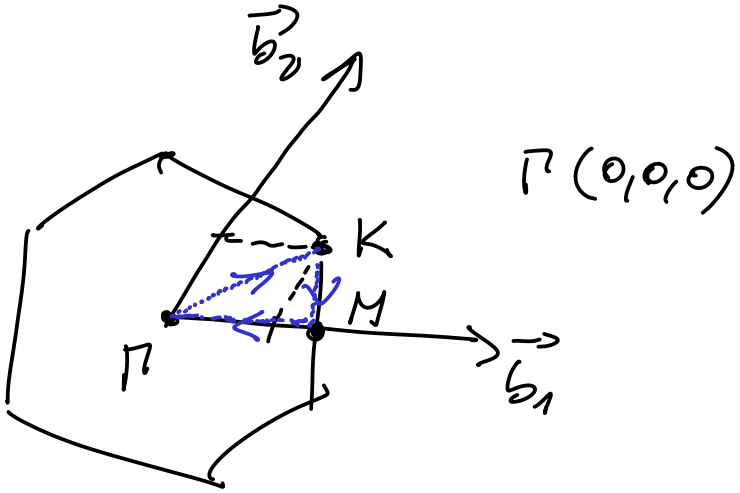


Benzene, an example of the D_{6h} point group:



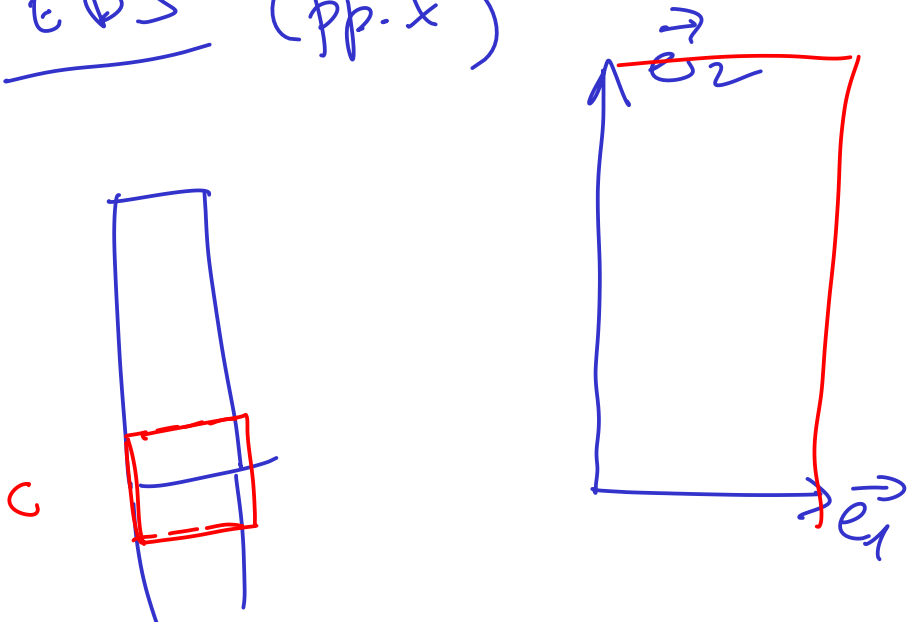
BANDS (scf) → (bands)

pw.x automatic crystal_b

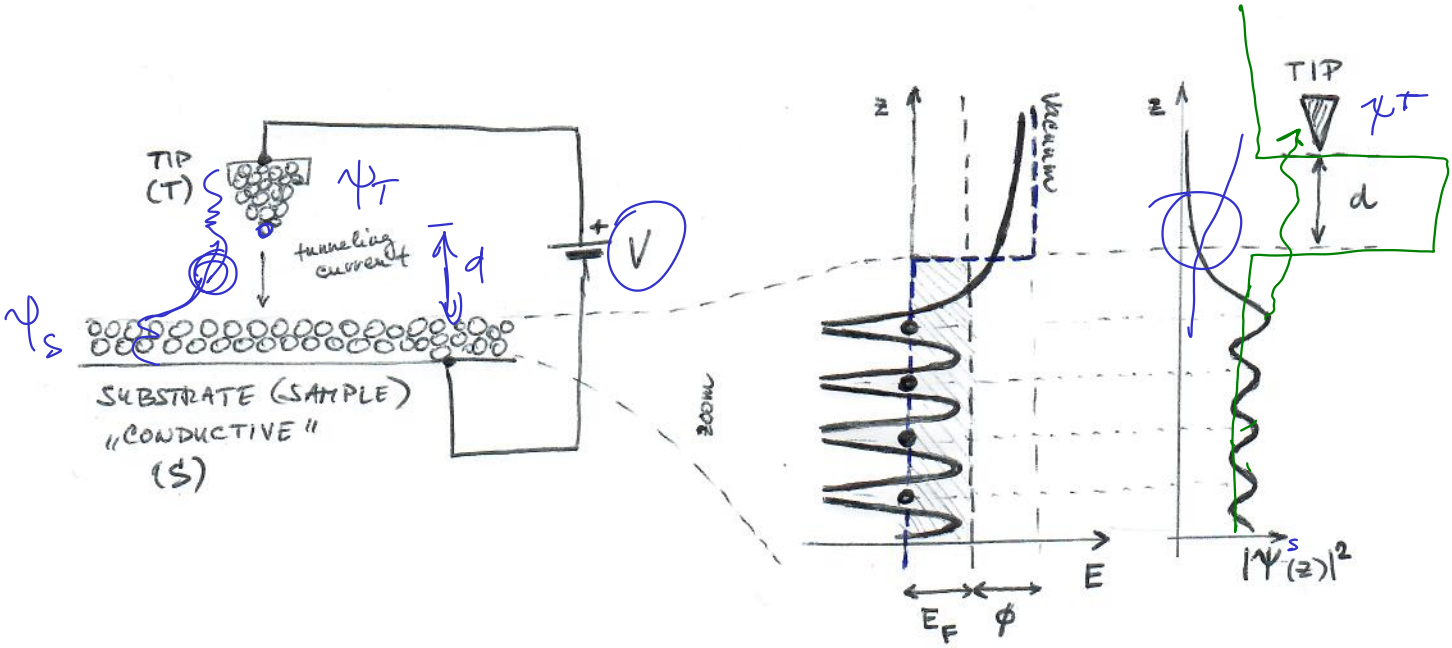


Γ (0,0,0)

DOS (pp.x)

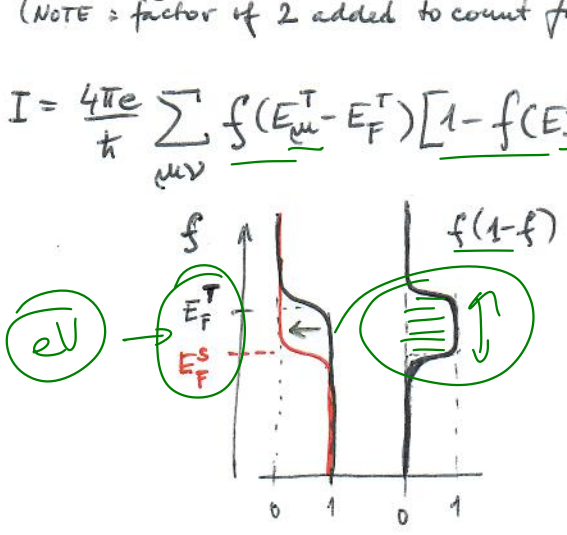


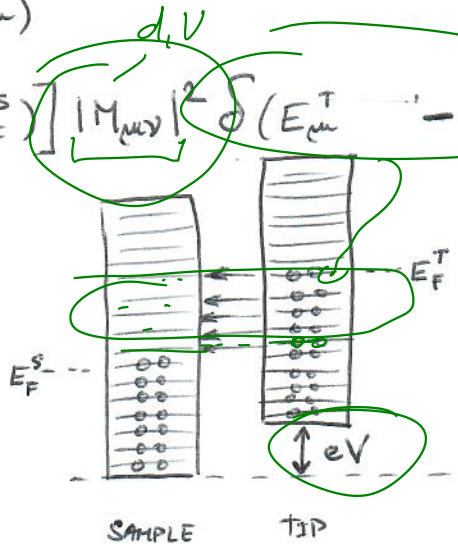
Scanning Tunneling Microscope (STM)



- electron can tunnel from an occupied state ψ^S_μ to an unoccupied state ψ^T_ν and vice-versa.
- at non-zero temperature the occupied states are given by Fermi-Dirac distribution $f(E-E_F) = \left[1+\exp\left((E-E_F)/k_BT\right)\right]^{-1}$ while unoccupied states are described by $1-f(E-E_F)$
- tunneling current in thermal equilibrium from tip to sample (Bardeen's expression) (NOTE: factor of 2 added to count for spin)

$$I = \frac{4\pi e}{\hbar}\sum_{\mu\nu} f(E^T_\mu - E^T_F)\left[1-f(E^S_\nu - E^S_F)\right]|M_{\mu\nu}|^2\,\delta(E^T_\mu - E^S_\nu)$$





$$\sum_\mu \longrightarrow \int \rho(\epsilon)\,d\epsilon$$

$$M_{\mu\nu} = \frac{1}{2}\int d\vec{S}\cdot\left(\psi^*_{T\mu}\nabla\psi_{S\nu} - \psi_{S\nu}\nabla\psi^*_{T\mu}\right)$$

matrix elements of the current operator (constructive interference of the wfcs in S and T)

$$E_F^T = E_F^S + eV$$

Tersoff–Hamann approximation — assumption of a spherical tip

$$M_{\mu\nu} = \text{const} \cdot \Psi^S_\nu(\vec{r}_T)$$

↳ centre of the sphere

Density of states for the tip

$$\rho^T(E) = \sum_\mu \delta(E - E^T_\mu)$$

$$I = \frac{4\pi e}{\hbar} \int dE\, \rho^T(E) f(E - E^S_F - eV)\left[1 - f(E - E^S_F)\right] \times \sum_\nu |\Psi^S_\nu(\vec{r}_T)|^2 \delta(E - E^S_\nu) \cdot \text{const}$$

in low-temperature limit $f(E) \longrightarrow \Theta(E)$

$$I = \text{const} \int_{E^S_F}^{E^S_F + eV} dE\, \rho^T(E) \times \sum_\nu |\Psi^S_\nu(\vec{r}_T)|^2 \delta(E - E^S_\nu)$$

assuming that $\rho^T(E)$ does not depend/change much with the energy

$$I \approx \text{const} \sum_{\nu:\, E^S_\nu > E^S_F}^{E^S_F + eV} |\Psi^S_\nu(\vec{r}_T)|^2$$

To calculate STM maps using DFT

$\Psi^S_\nu(\vec{r}) = \phi_\nu(\vec{r})$ Kohn–Sham eigenstate

$E^S_\nu = \varepsilon_\nu$ Kohn–Sham eigenvalue