

$$-\frac{\hbar}{2m} \frac{\partial^2 \Psi(x)}{\partial x^2} = E \Psi(x) \quad \text{for } x > a$$

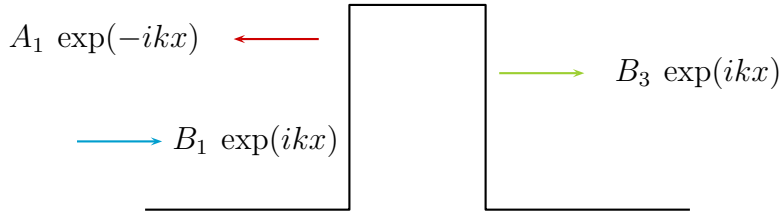
$$-\frac{\hbar}{2m} \frac{\partial^2 \Psi(x)}{\partial x^2} + U_0 \Psi(x) = E \Psi(x) \quad \text{for } 0 < x < a$$

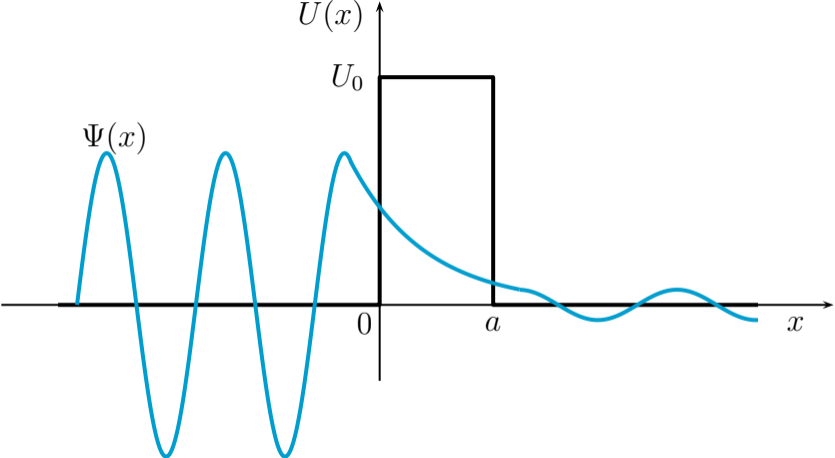
$$-\frac{\hbar}{2m} \frac{\partial^2 \Psi(x)}{\partial x^2} = E \Psi(x) \quad \text{for } x < 0$$

$$\Psi(x) = A_1 \exp(-i kx) + B_1 \exp(i kx)$$



$$\Psi(x) = A_3 \exp(-i kx) + B_3 \exp(i kx)$$





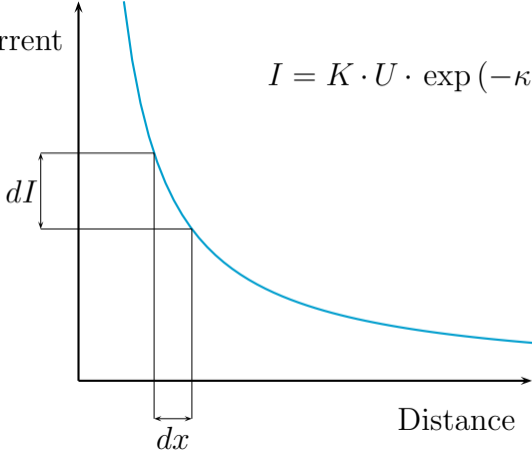
Current

$$I = K \cdot U \cdot \exp(-\kappa \cdot x)$$

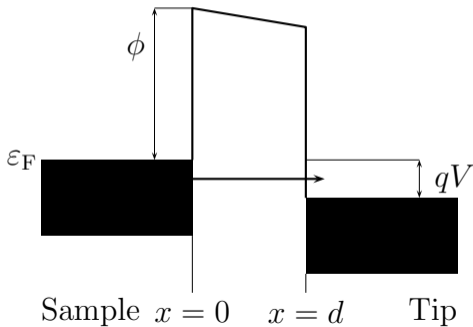
$dI$

$dx$

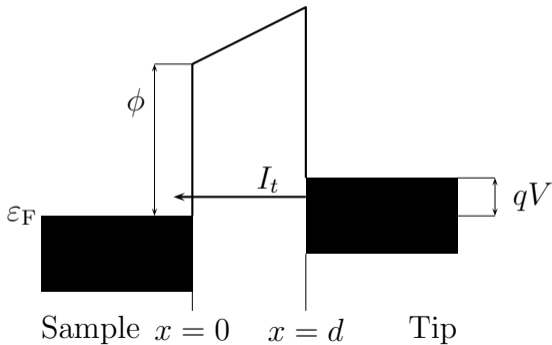
Distance



$V_{\text{bias}} < 0$  Vacuum

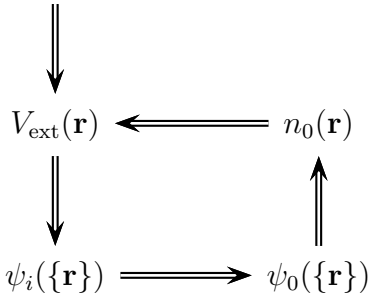


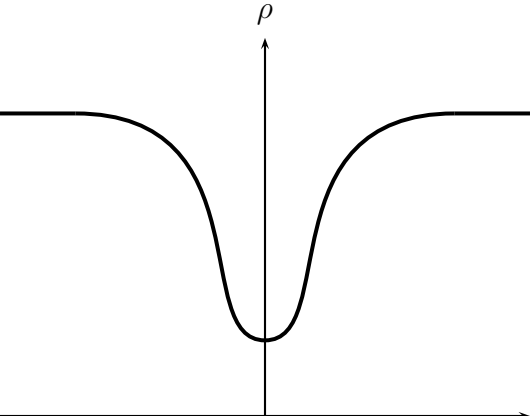
$V_{\text{bias}} > 0$  Vacuum



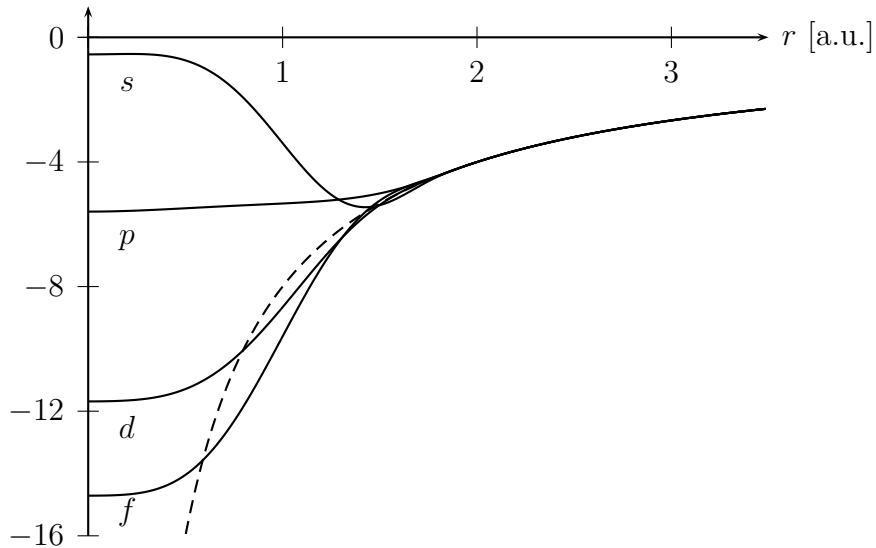


Guess of  $n_0(\mathbf{r})$

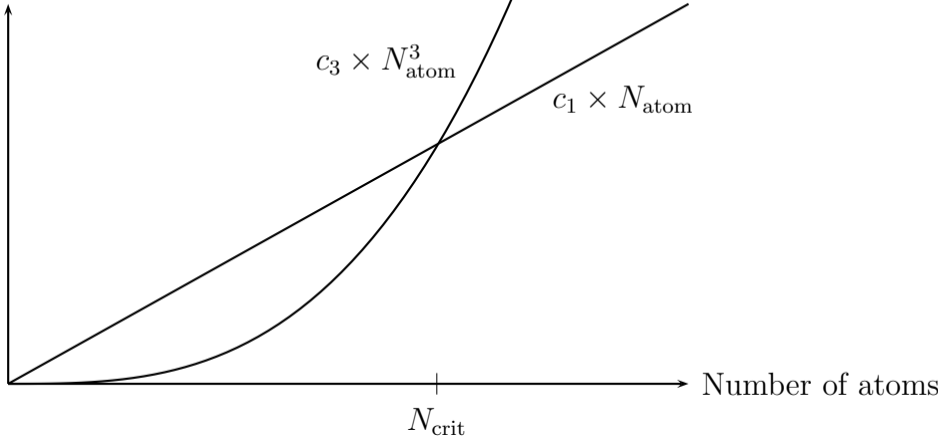




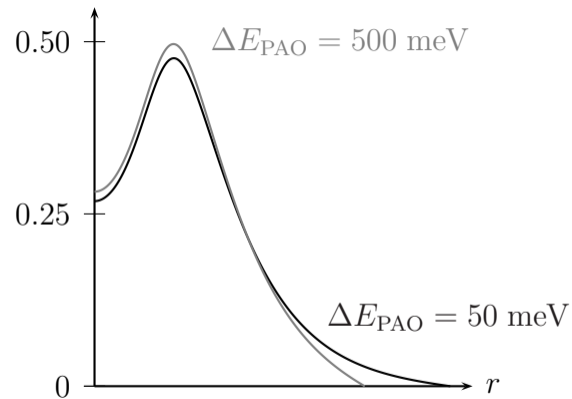
Potential [a.u.]



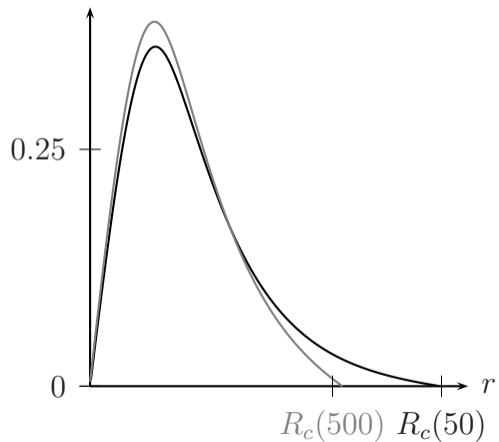
Computation time



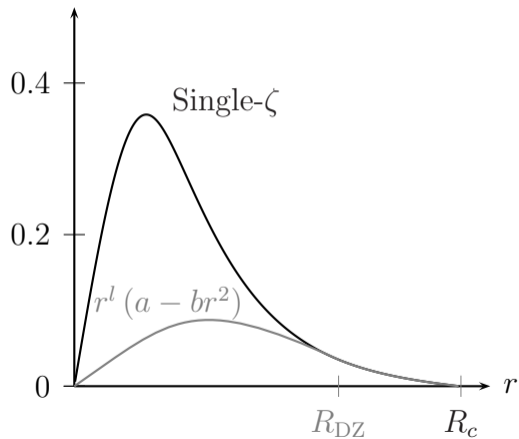
$\phi(r)$ , s-orbital



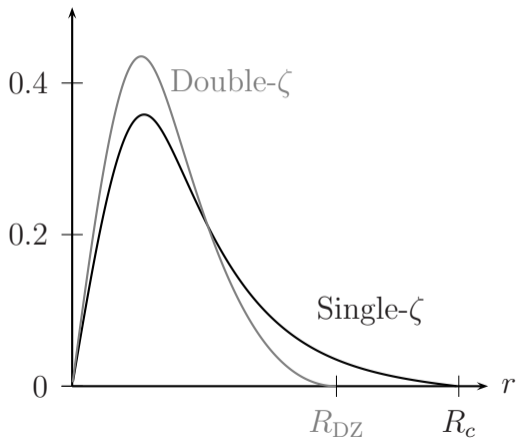
$\phi(r)$ , p-orbital

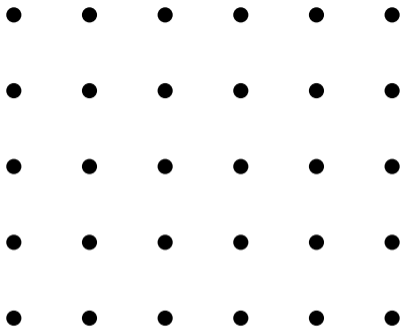


$\phi(r)$ , p-orbital



$\phi(r)$ , p-orbital



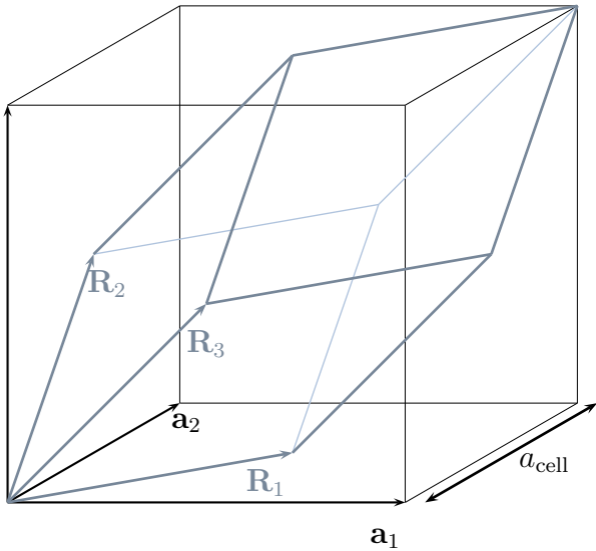


$\Delta x$

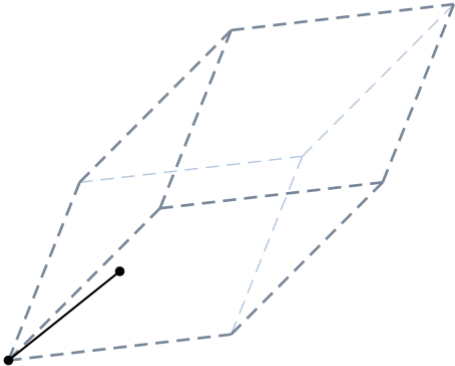
$$k_c = \frac{\pi}{\Delta x}$$

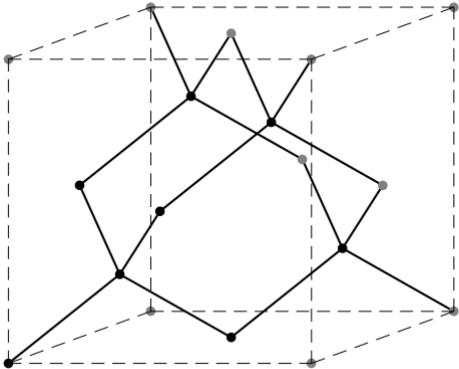
$$E_{\text{cut}} = \frac{\hbar^2 k_c^2}{2}$$



$\mathbf{a}_3$  $\mathbf{a}_2$  $\mathbf{R}_2$  $\mathbf{R}_3$  $\mathbf{R}_1$  $\mathbf{a}_1$  $a_{\text{cell}}$



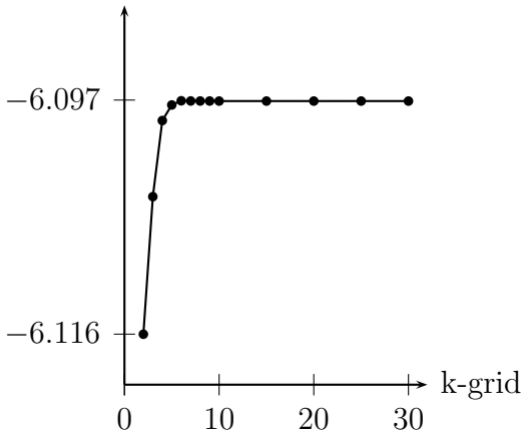


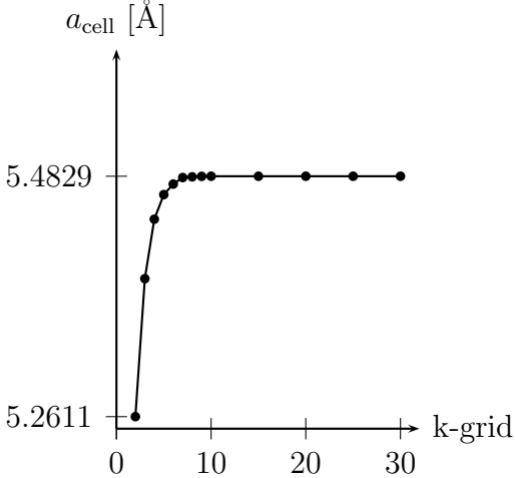


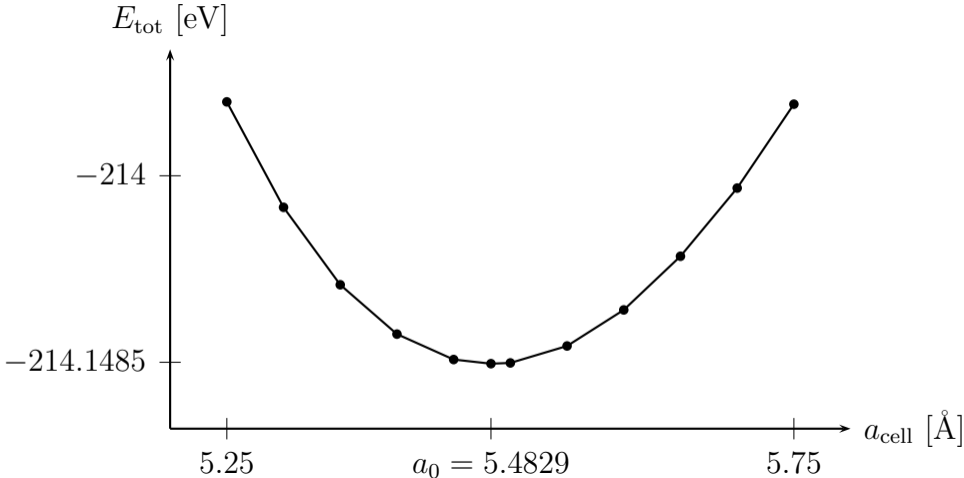


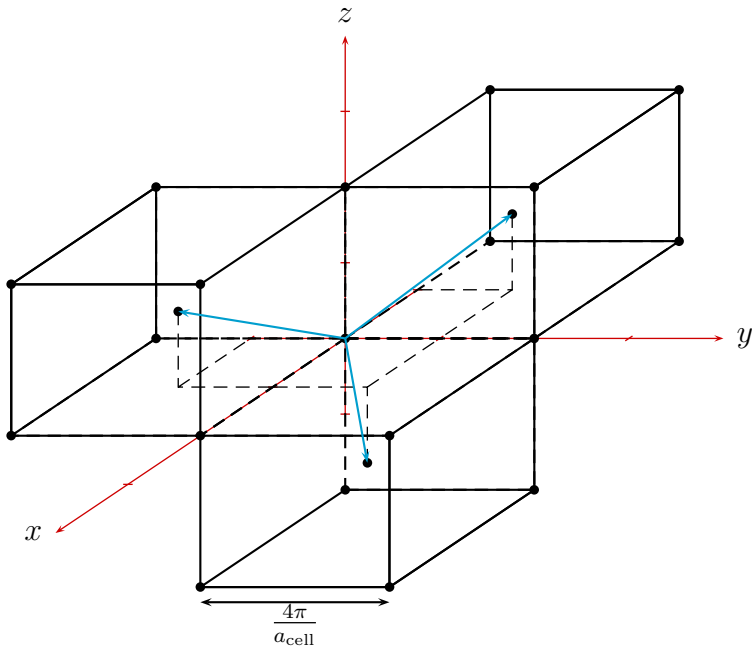


Cohesion Energy [eV]

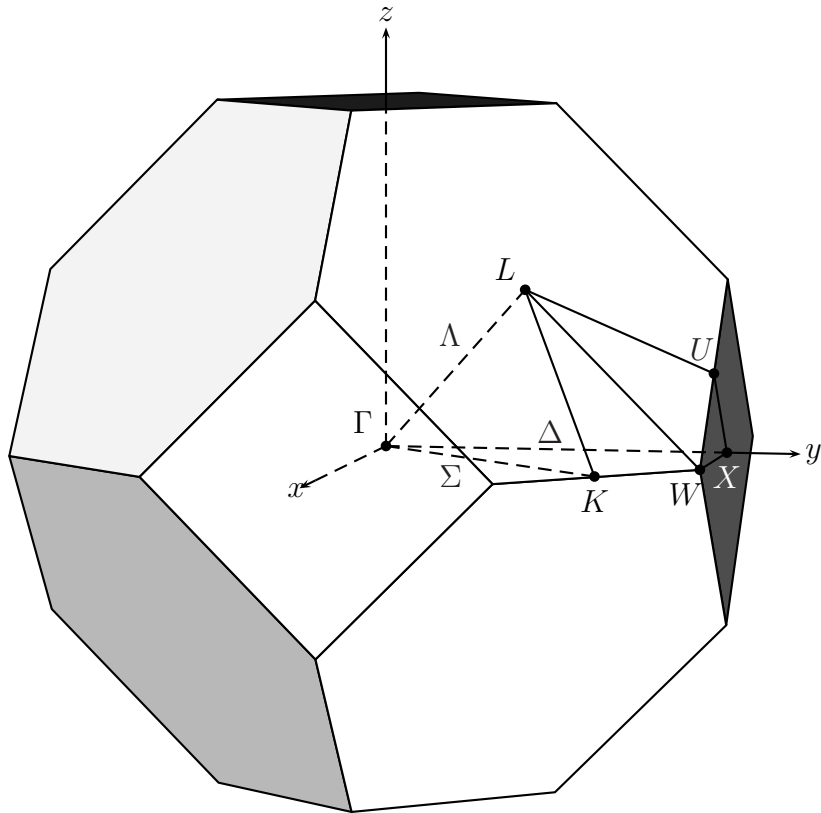


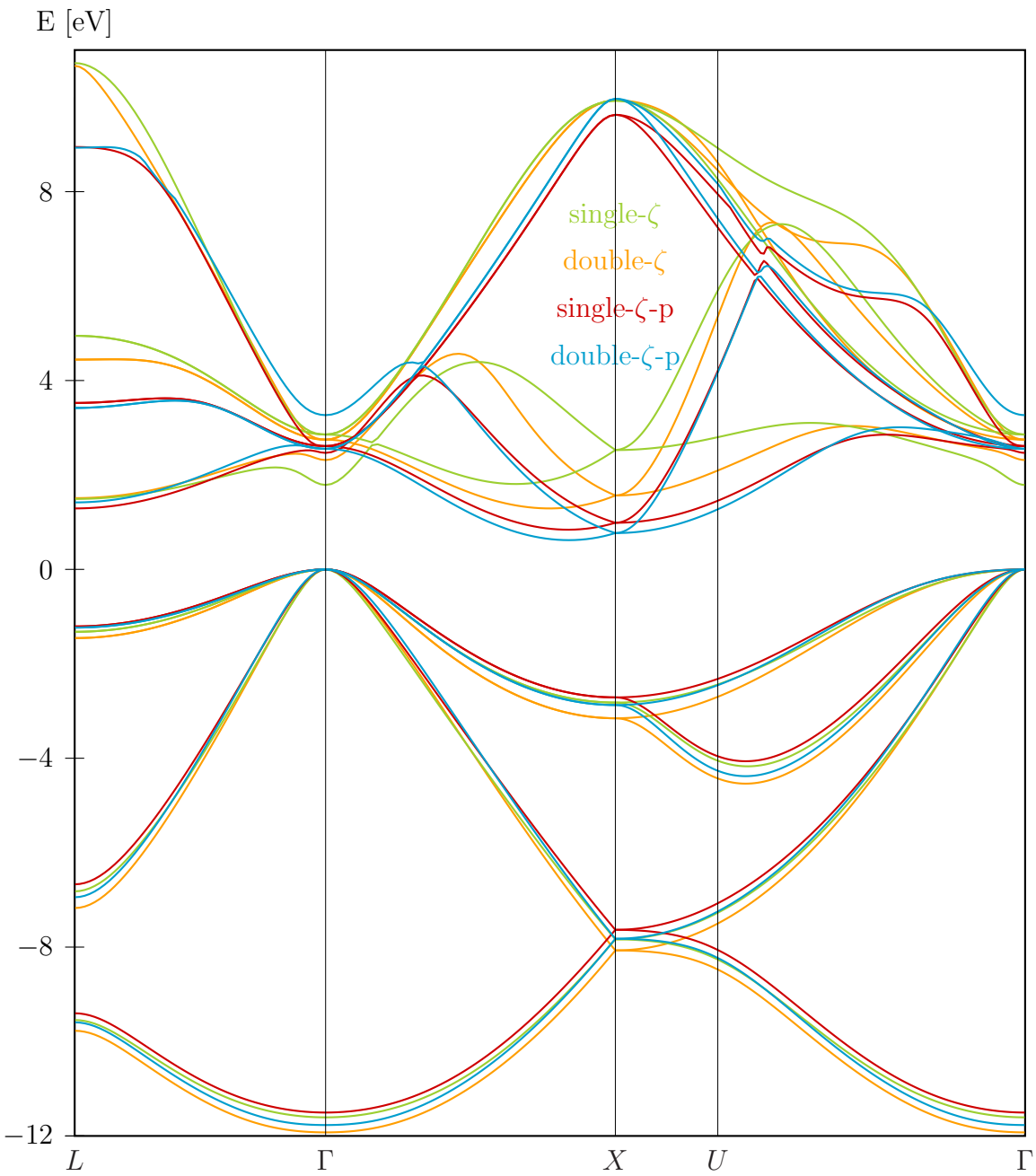


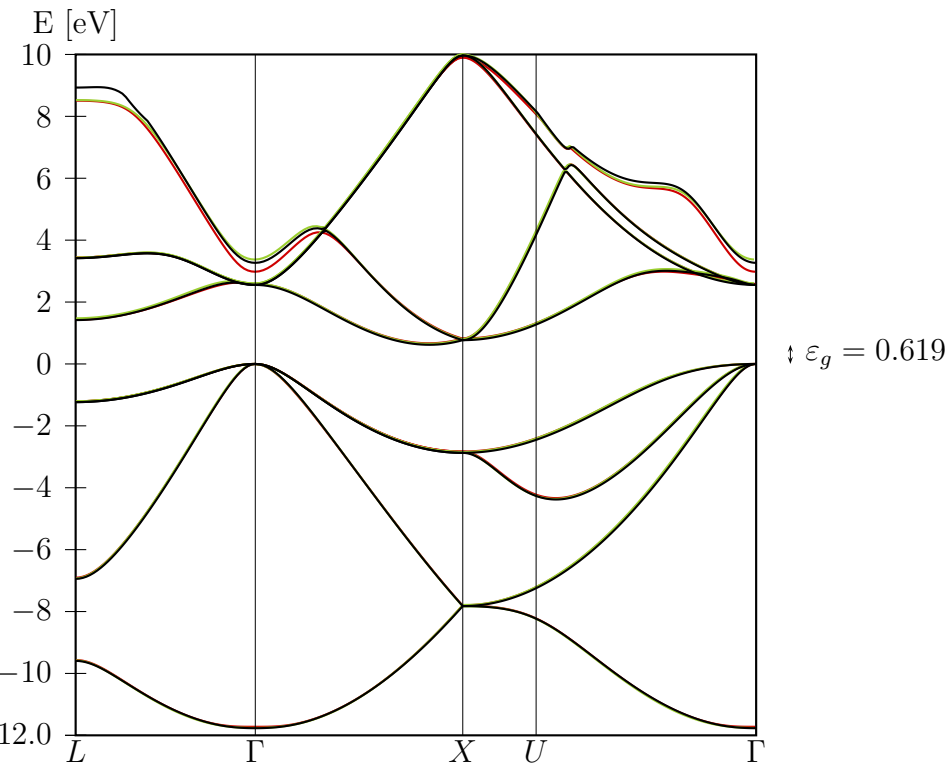


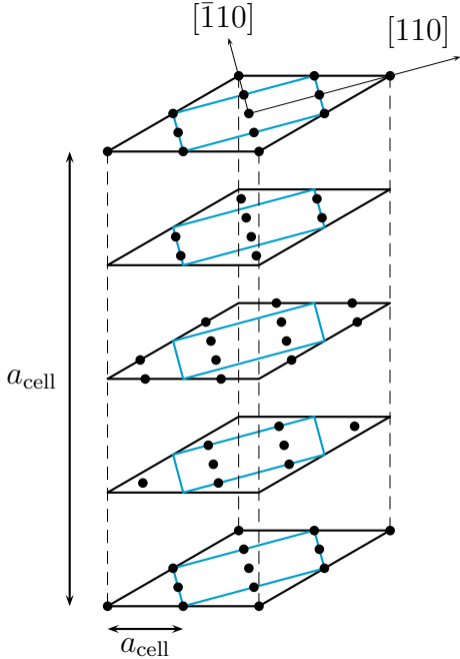


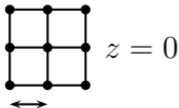
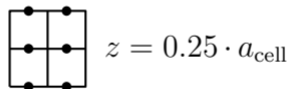
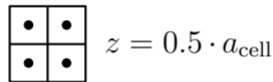
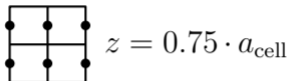
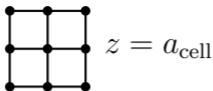










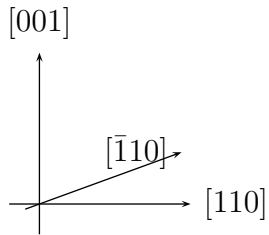
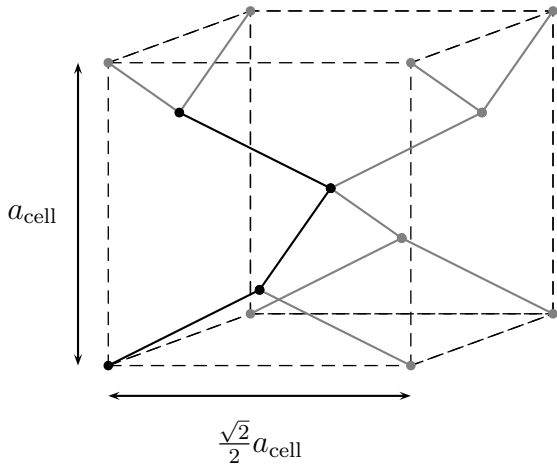


$[\bar{1}10]$

$[110]$

$\frac{\sqrt{2}}{2} a_{\text{cell}}$

$\frac{\sqrt{2}}{2} a_{\text{cell}}$



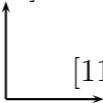


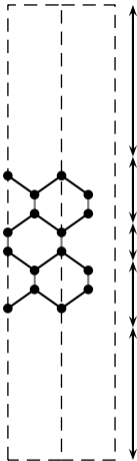
Adding free volume



$[001]$

$[110]$





Free volume

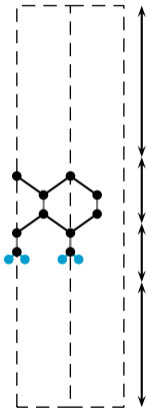
Relaxed

Fixed

Relaxed

Free volume



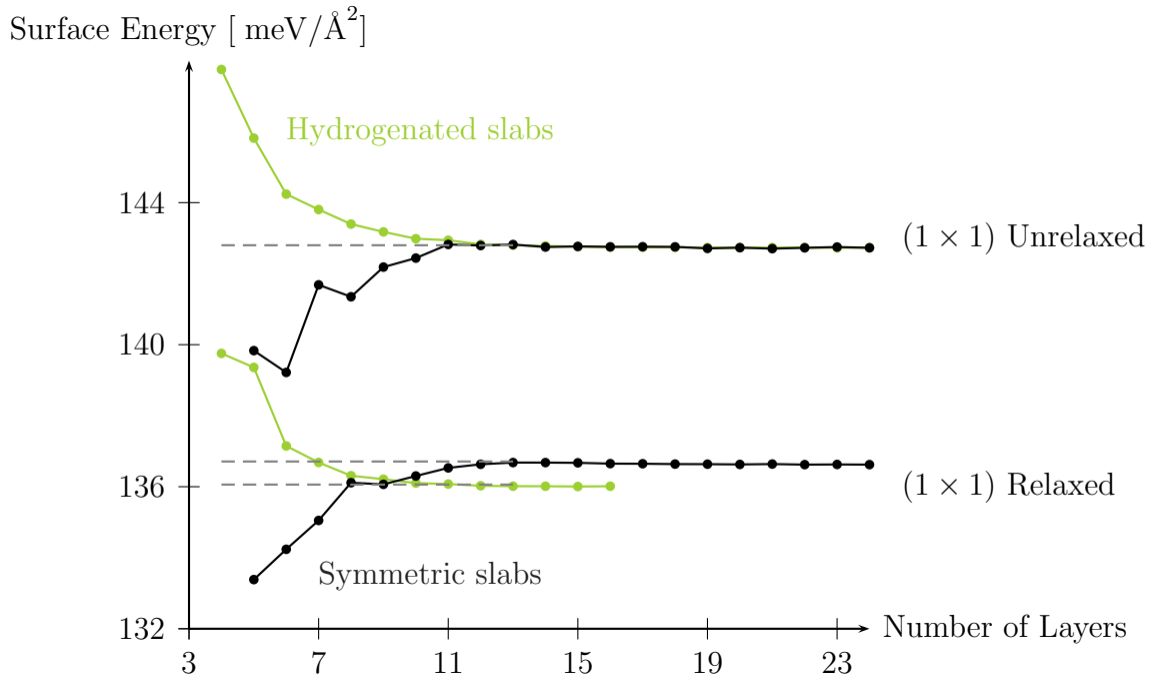


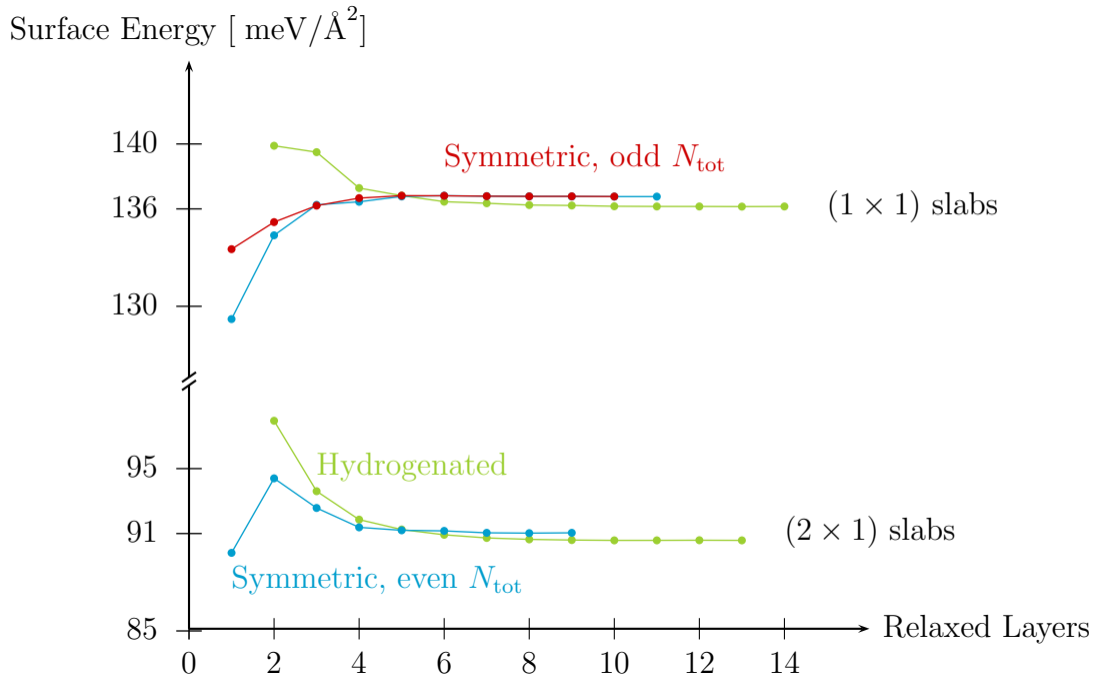
Free volume

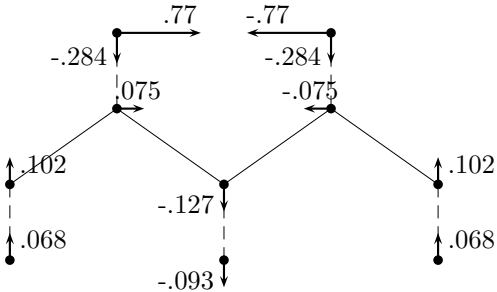
Relaxed

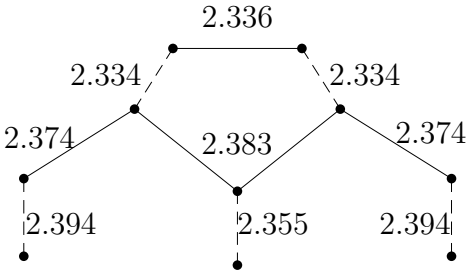
Fixed, with hydrogens

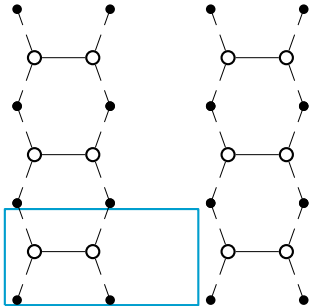
Free volume









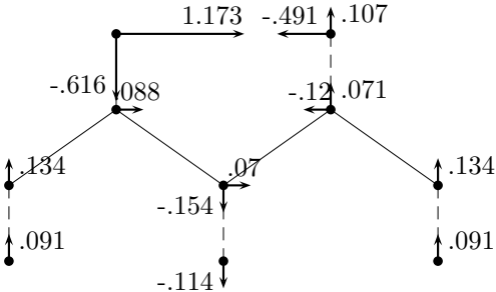


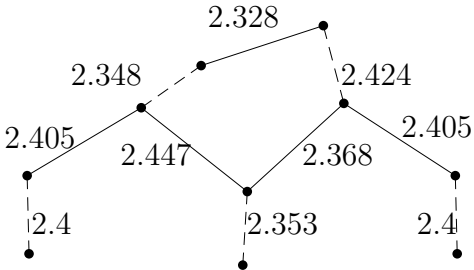
$[\bar{1}10]$



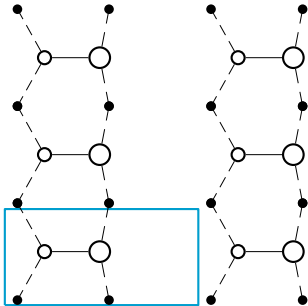
$[110]$









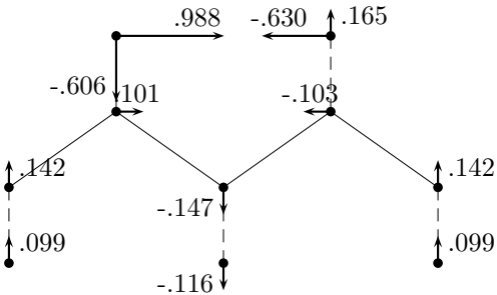


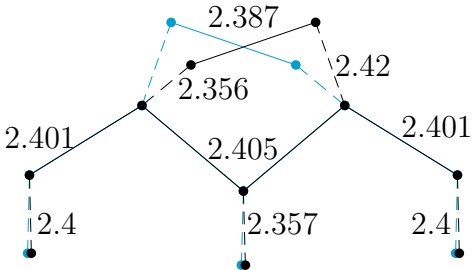
$[\bar{1}10]$

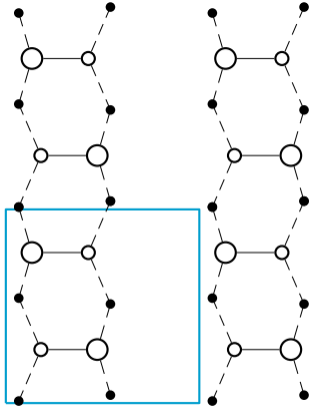


$[110]$

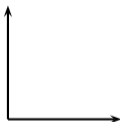




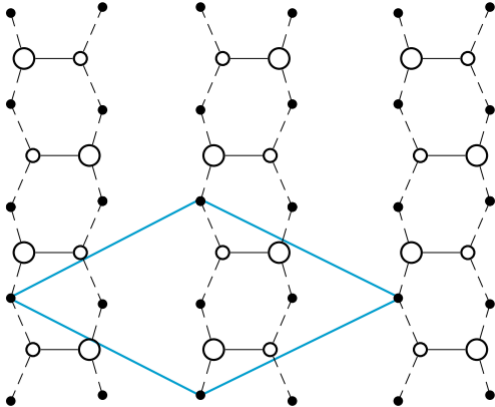




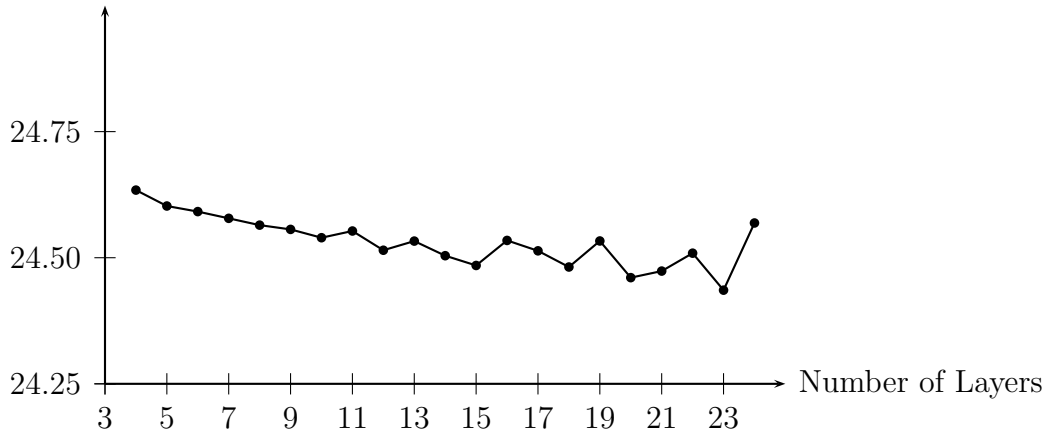
$[\bar{1}10]$

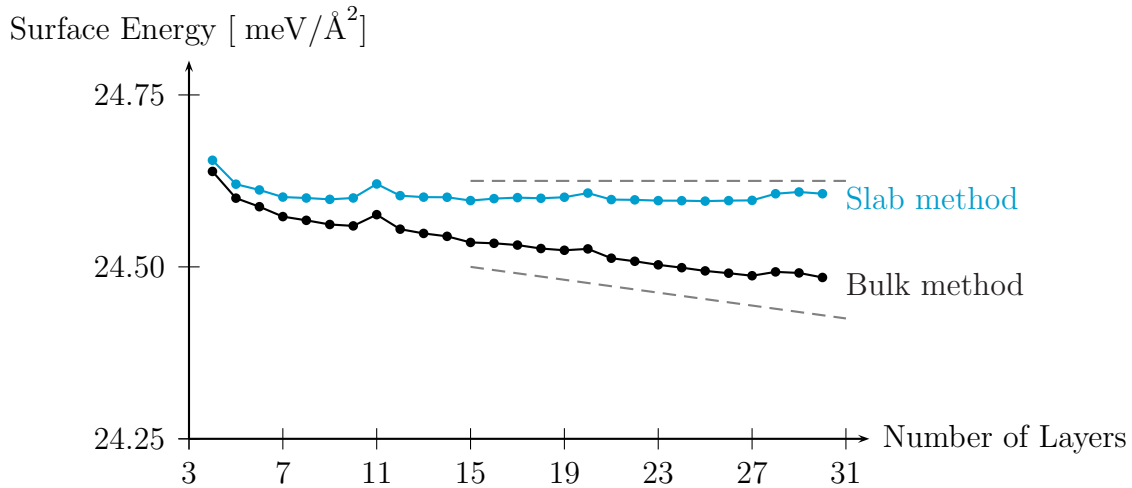


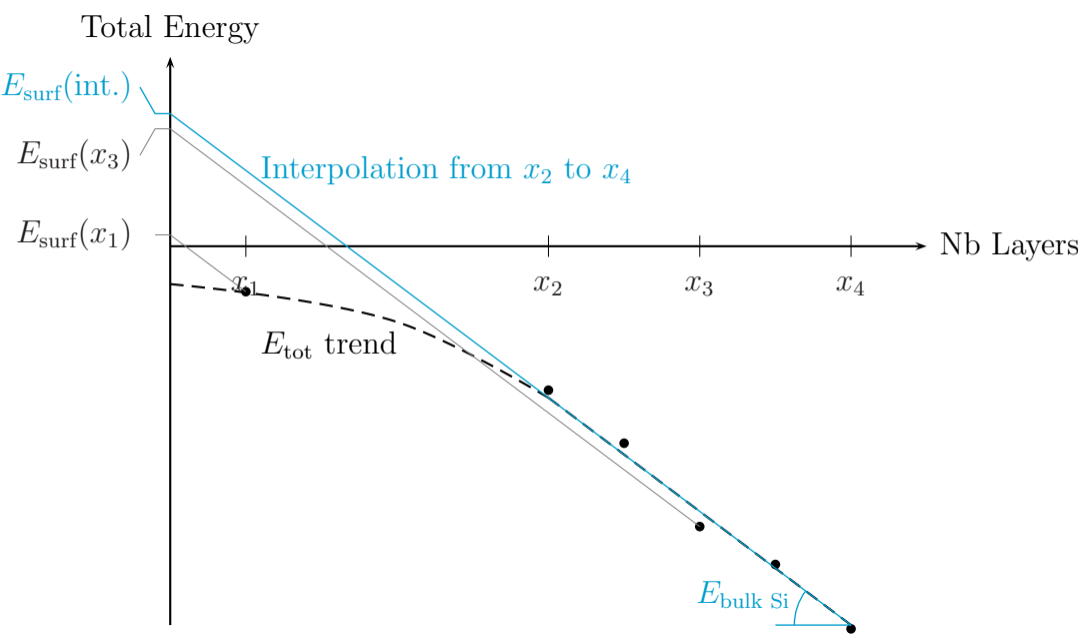
$[110]$



Surface Energy [ meV/Å<sup>2</sup>]

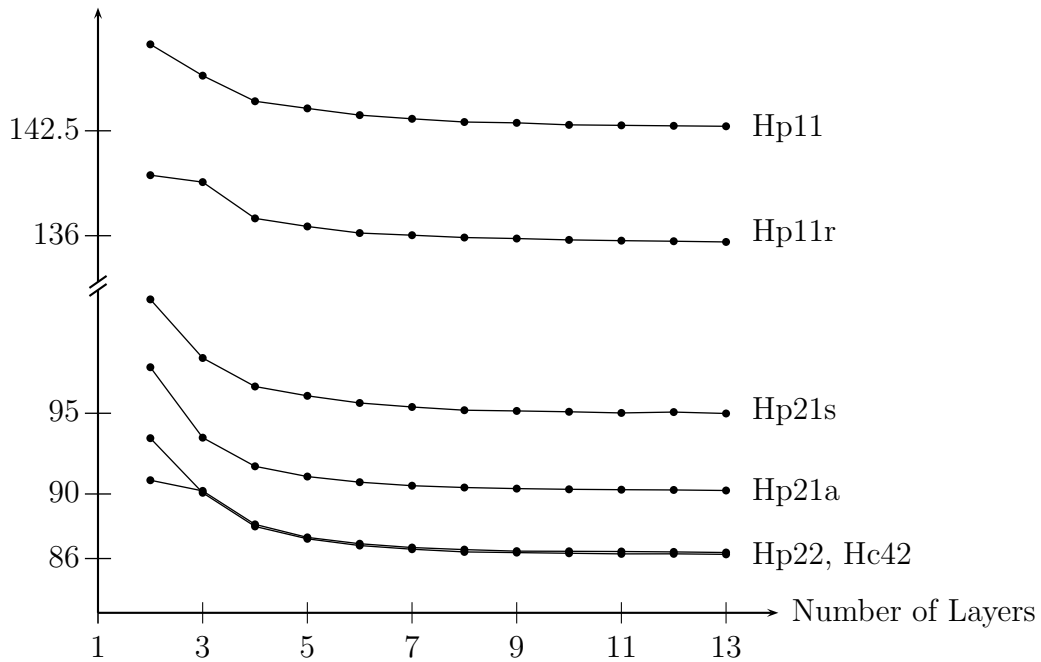


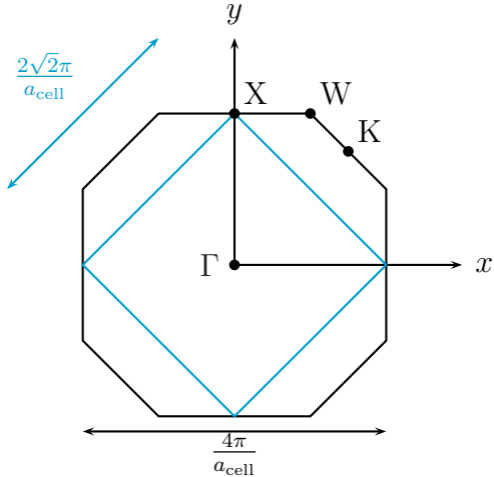


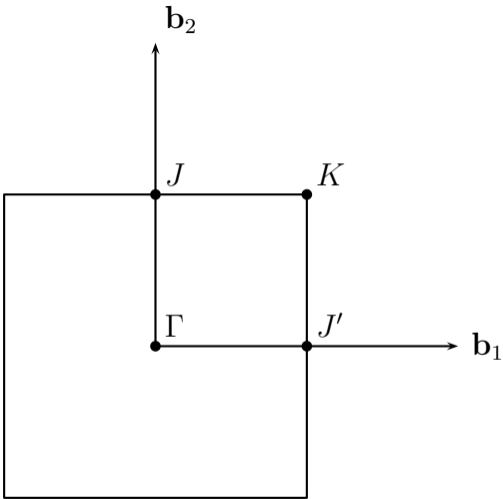


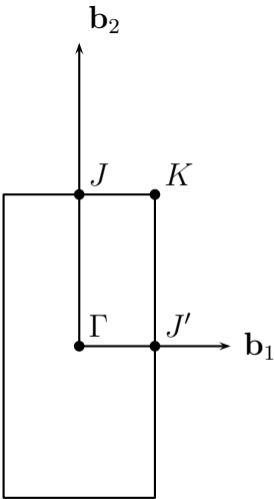


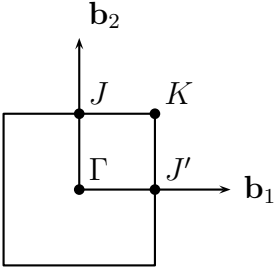
Surface Energy [ meV/Å<sup>2</sup>]

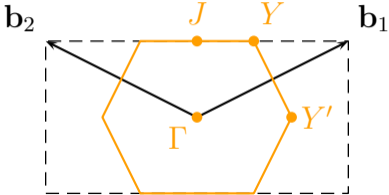


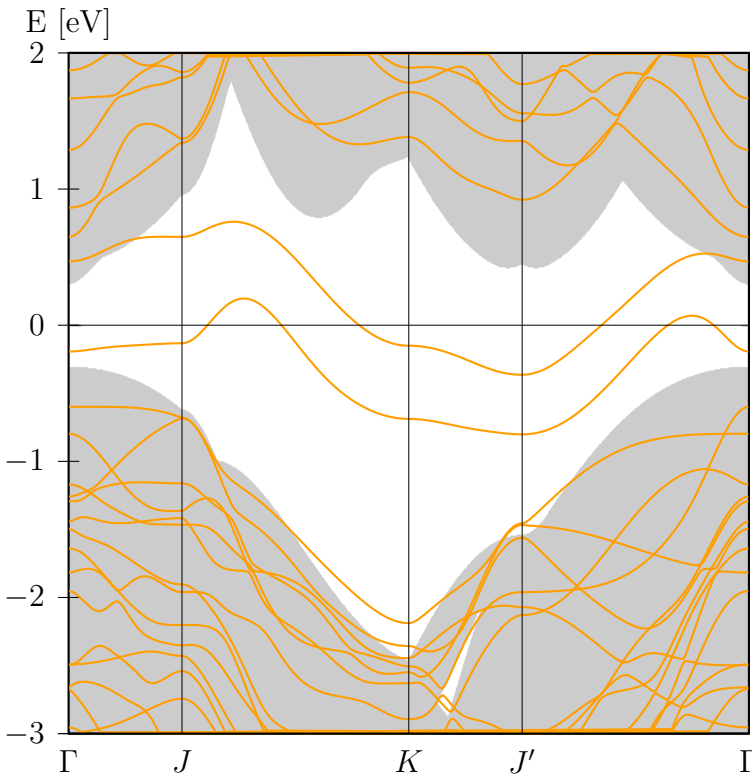




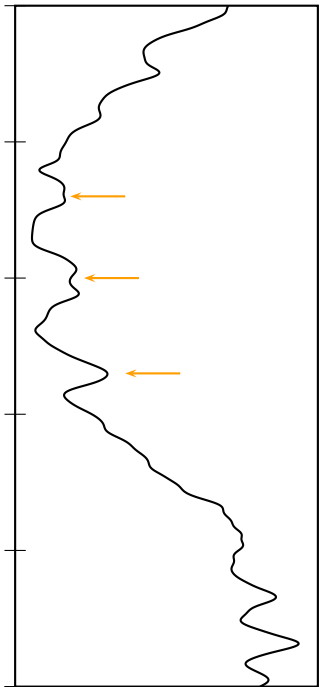




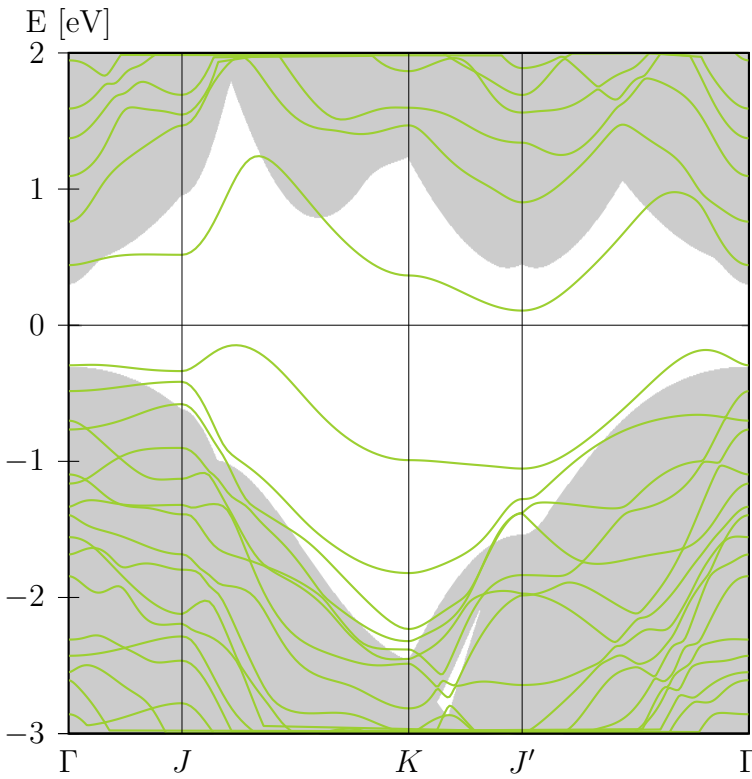




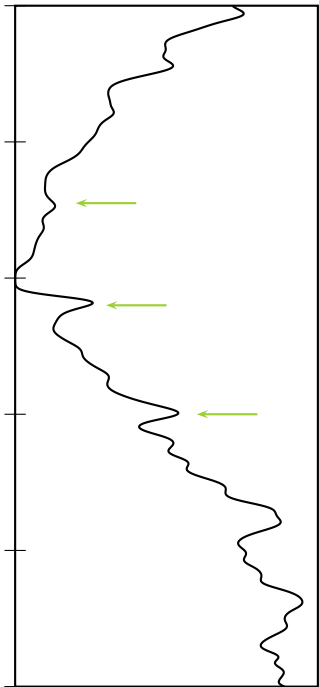
DOS [a.u.]

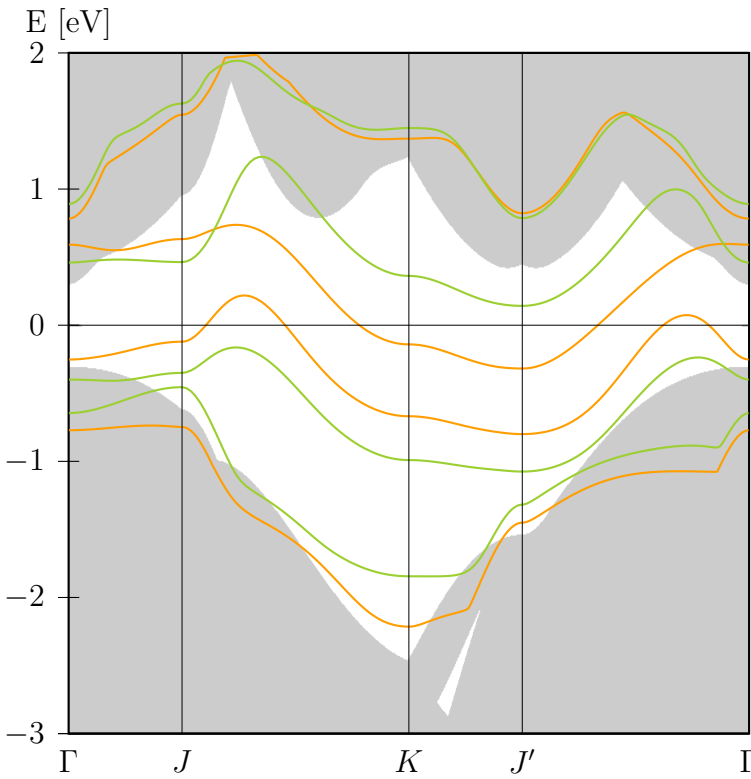


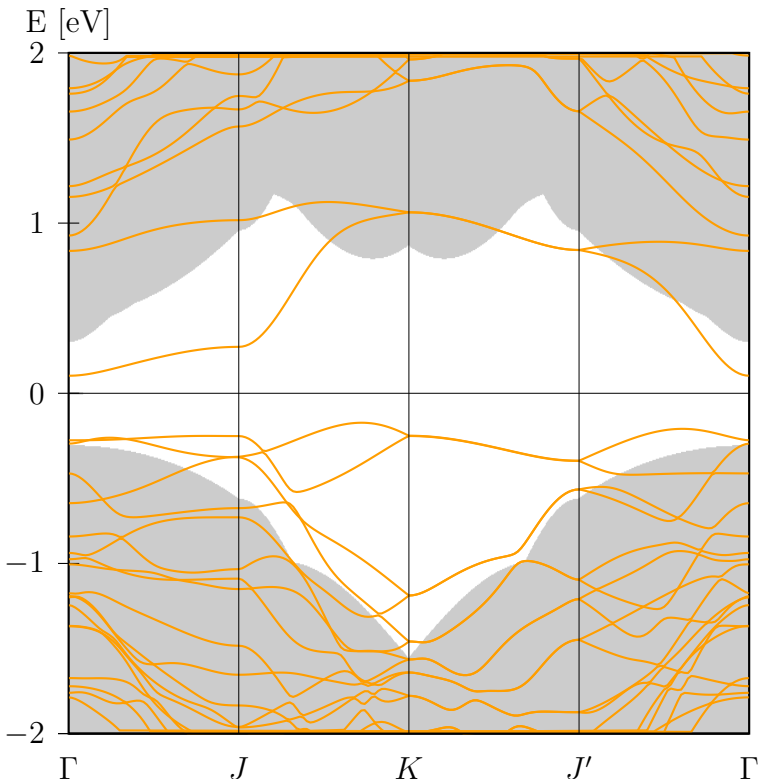




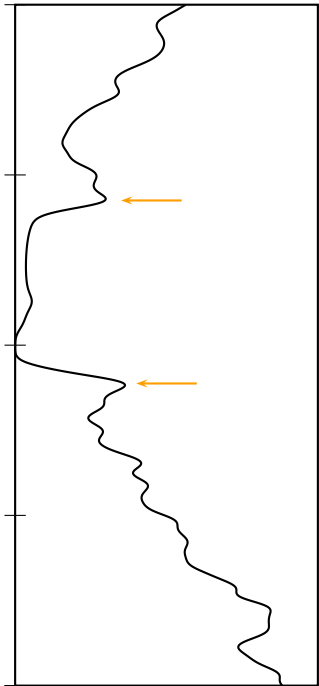
DOS [a.u.]

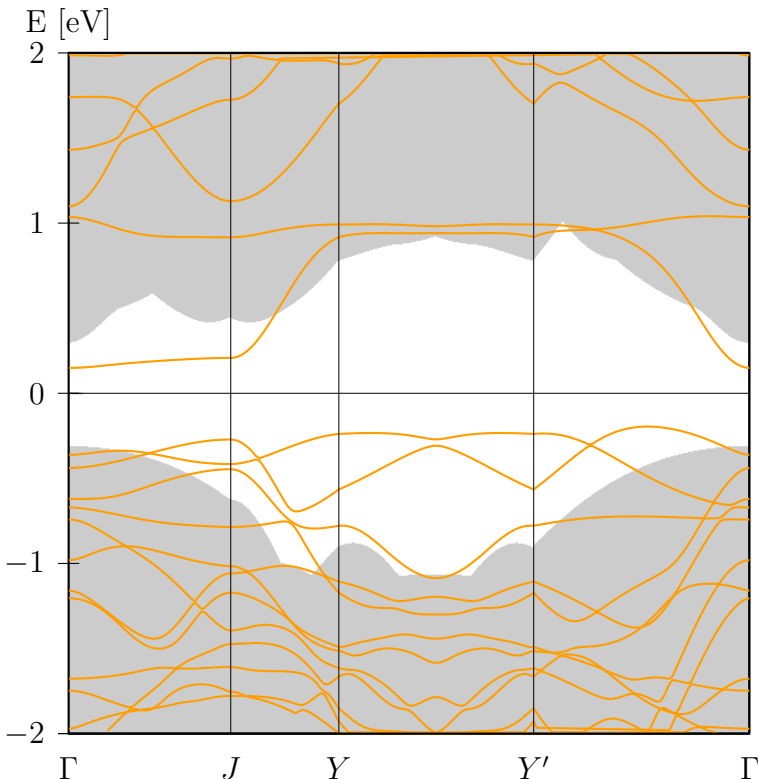




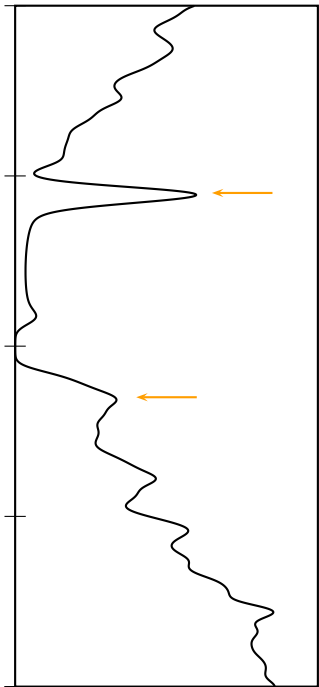


DOS [a.u.]

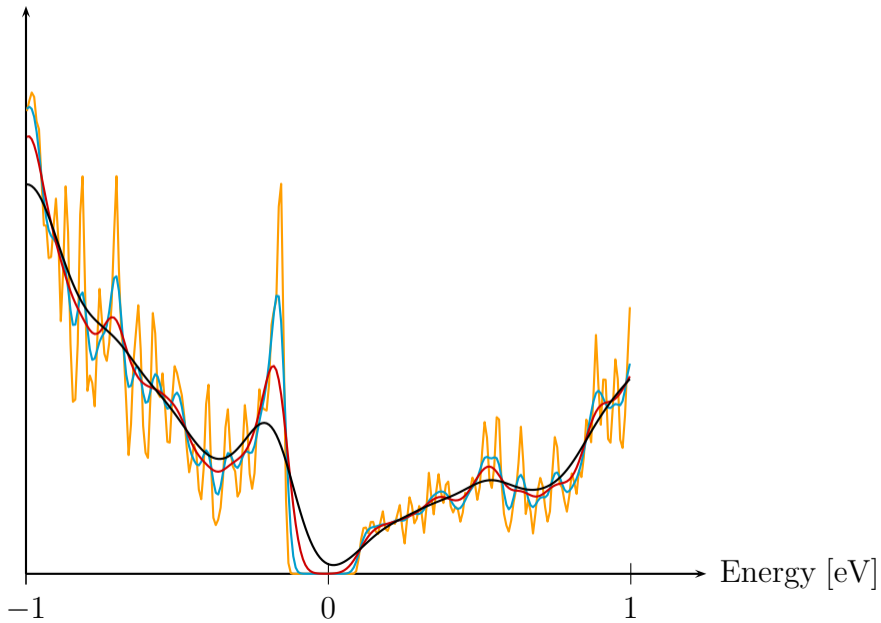




DOS [a.u.]

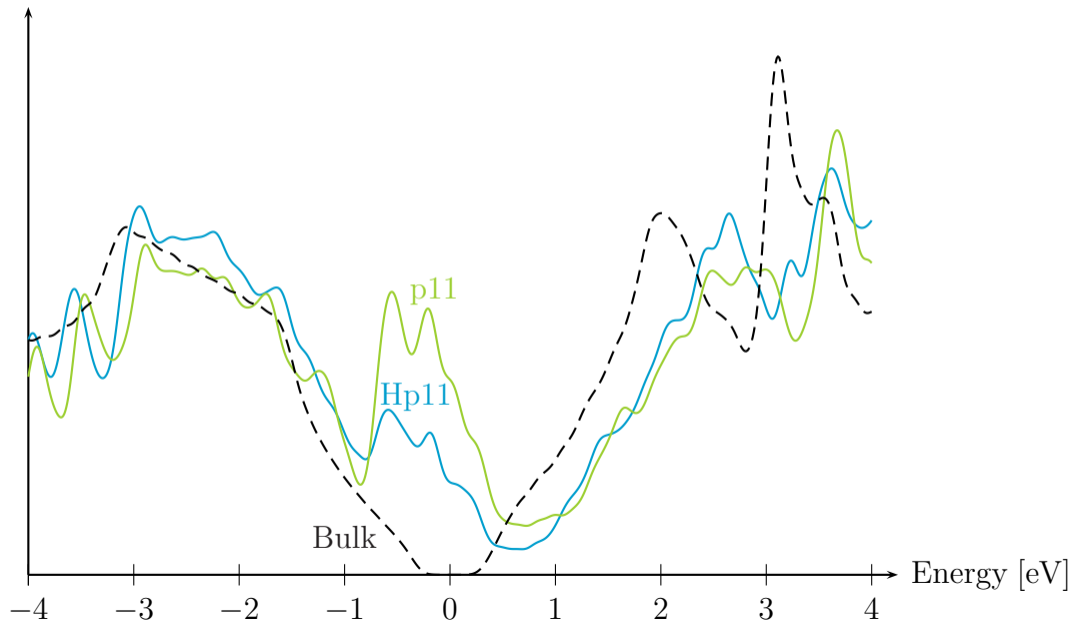


DOS [a.u.]

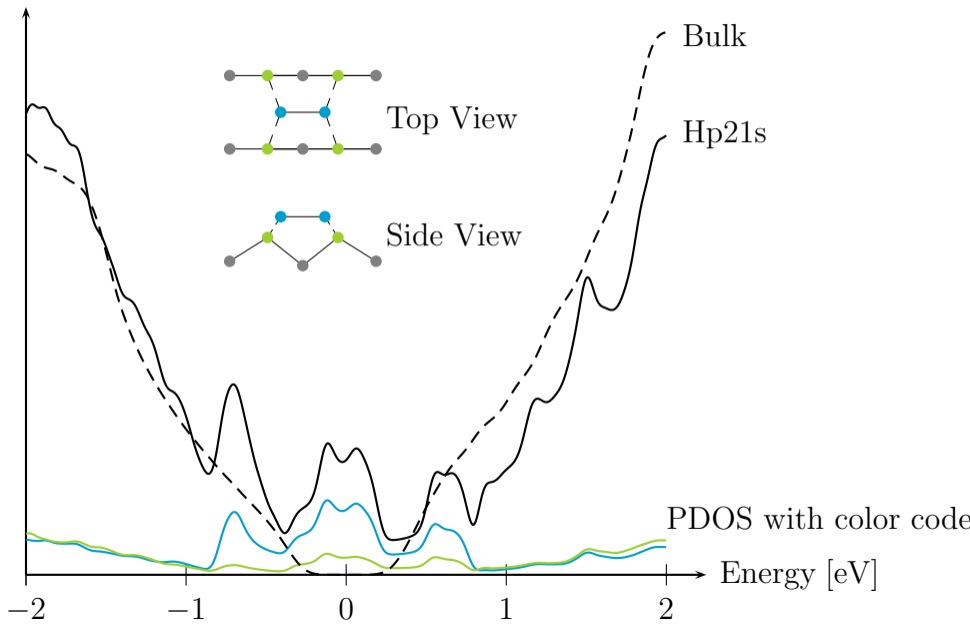




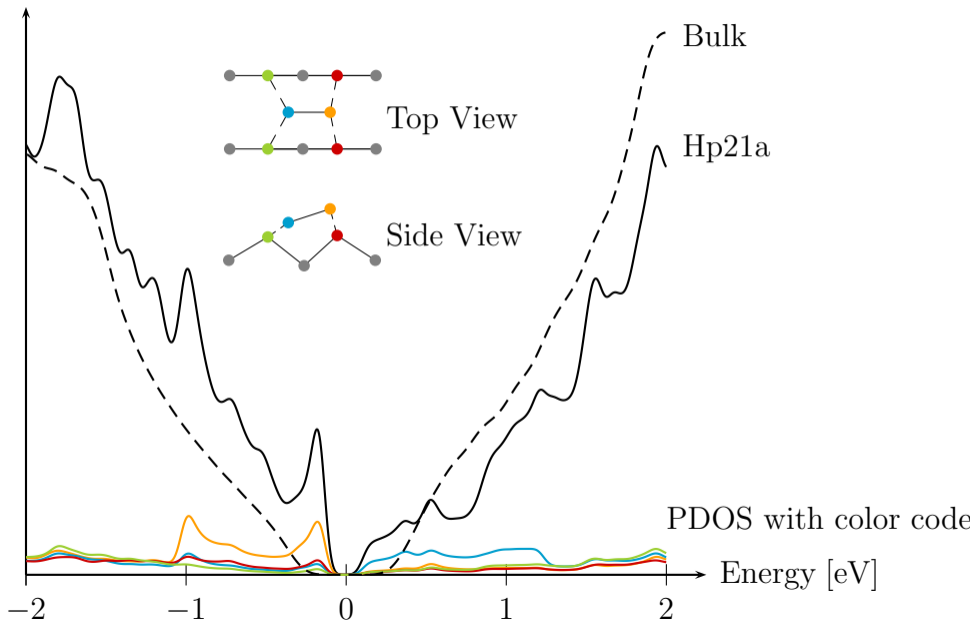
DOS [a.u.]



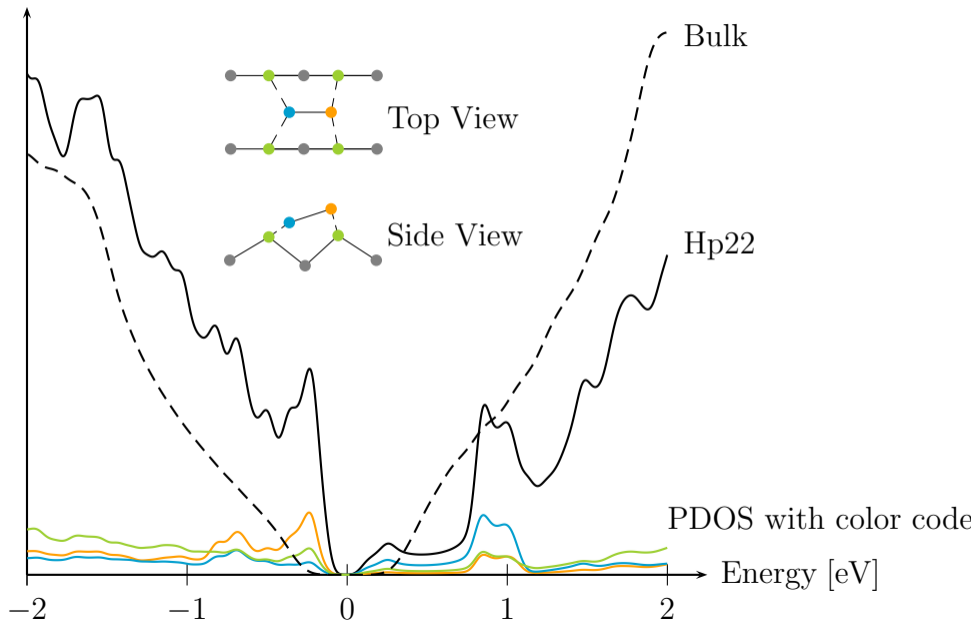
(P)DOS [a.u.]



(P)DOS [a.u.]



(P)DOS [a.u.]



(P)DOS [a.u.]

