

Sample

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

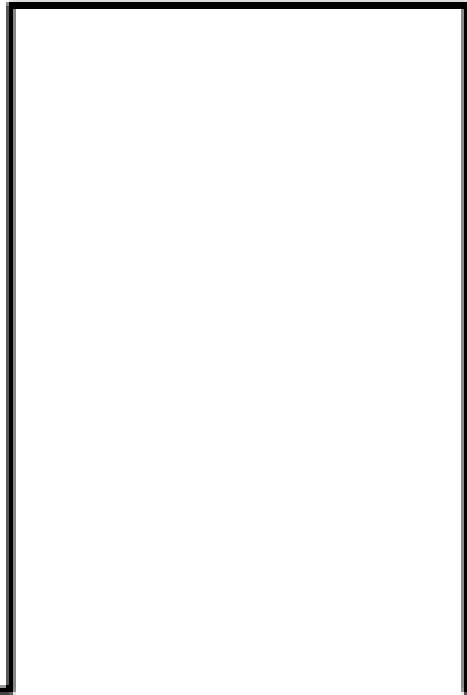
$$-\frac{\hbar}{2m} \frac{\partial^2 \Psi(x)}{\partial x^2} + U_0 \Psi(x) = E \Psi(x) \quad \text{for } 0 < x < a$$

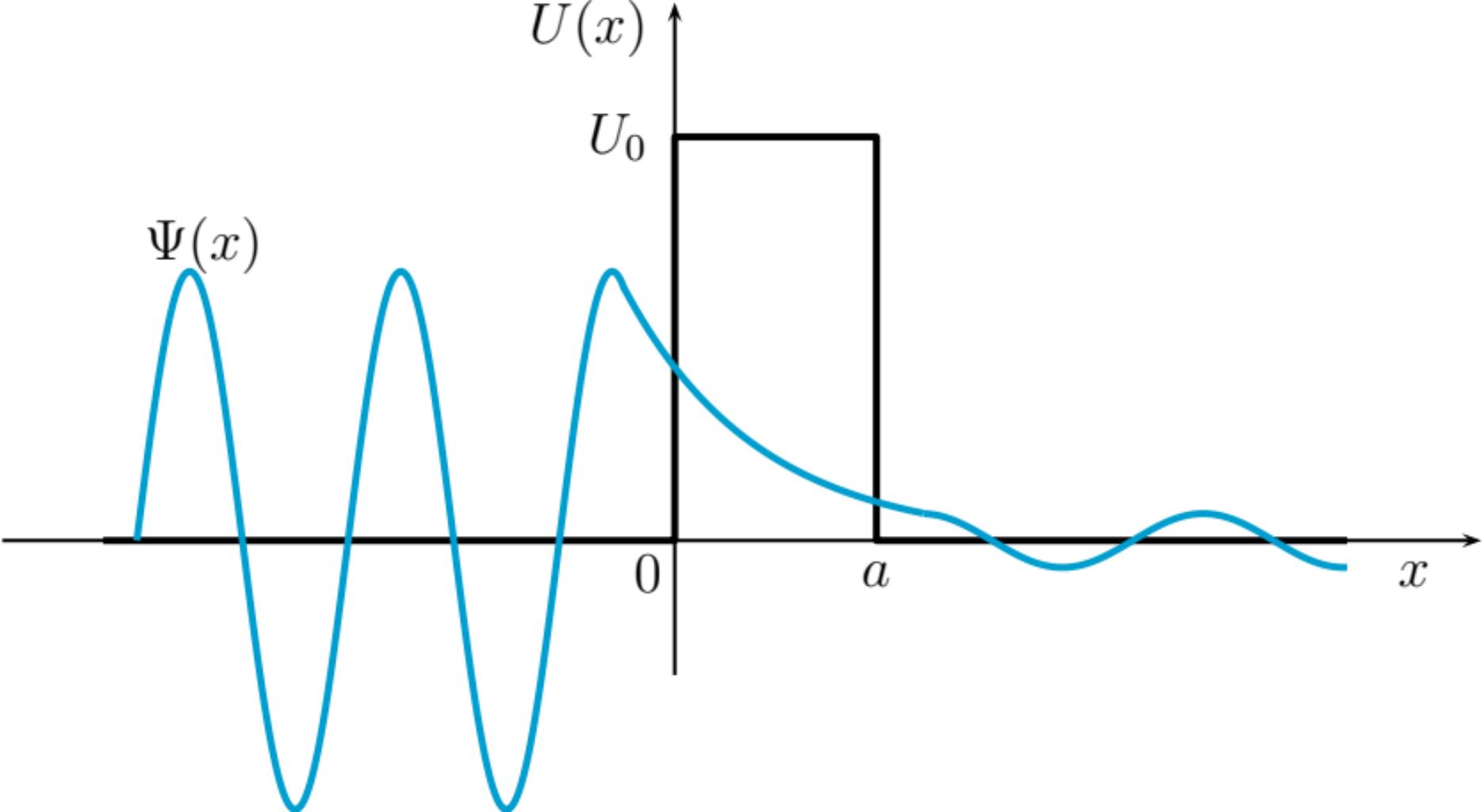
$$-\frac{\hbar}{2m} \frac{\partial^2 \Psi(x)}{\partial x^2} = E \Psi(x) \quad \text{for } x < 0$$

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



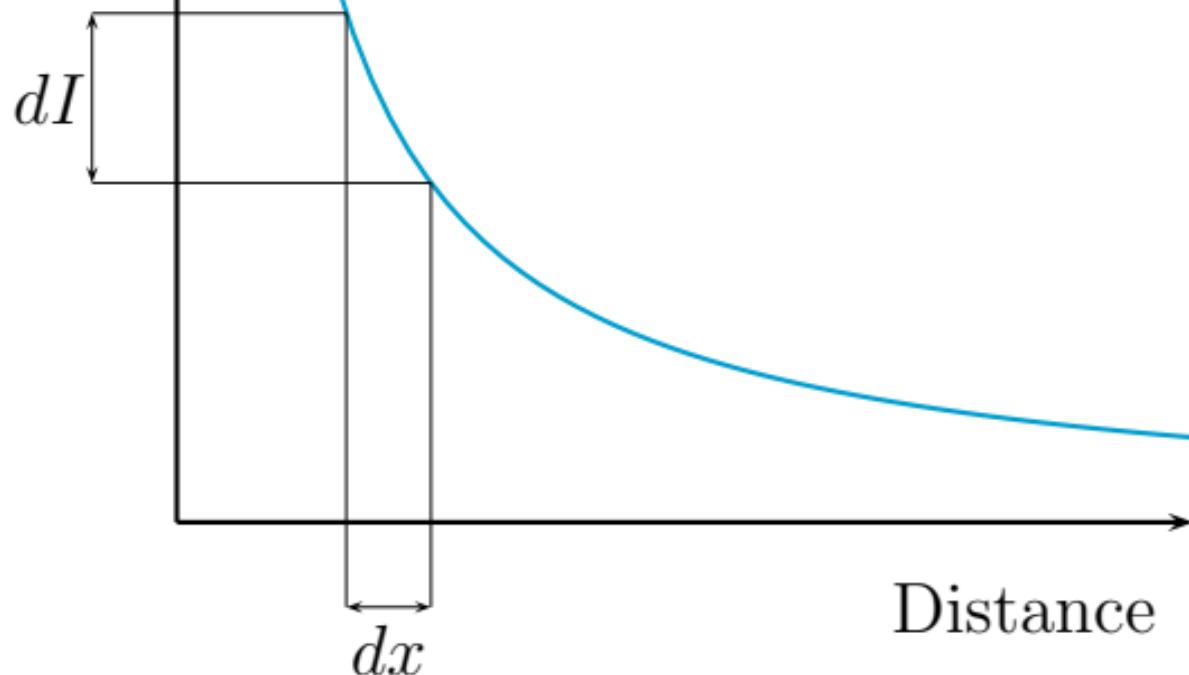
$$\Psi(x) = A_3 \exp(-i kx) + B_3 \exp(i kx)$$

$A_1 \exp(-ikx)$  $B_1 \exp(ikx)$  $B_3 \exp(ikx)$

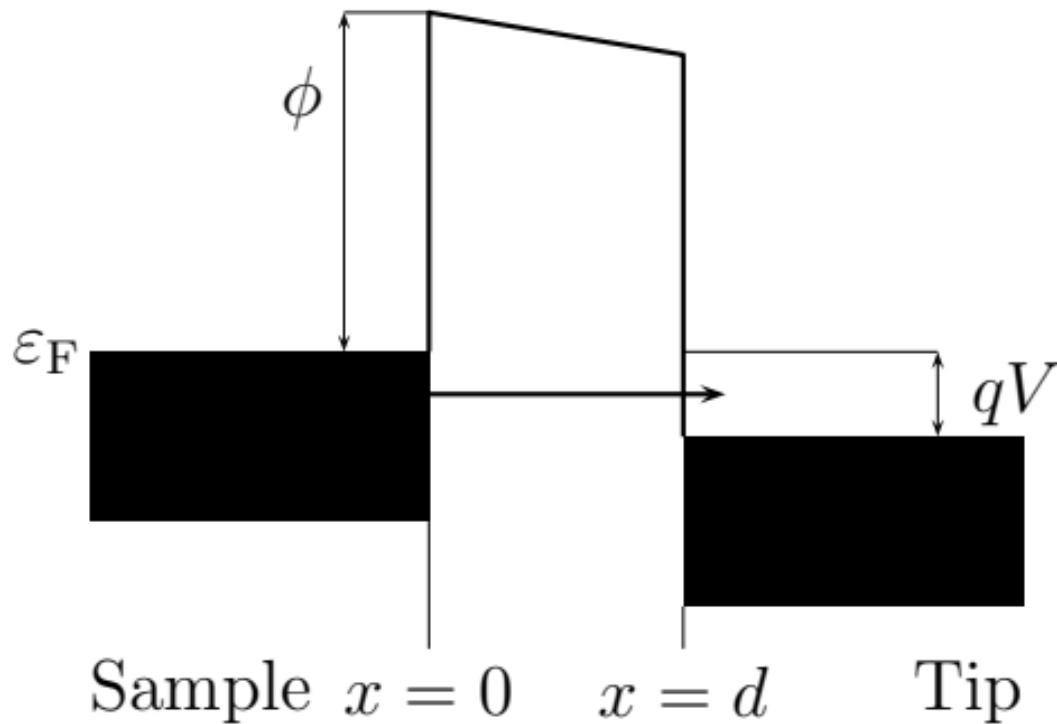


Current

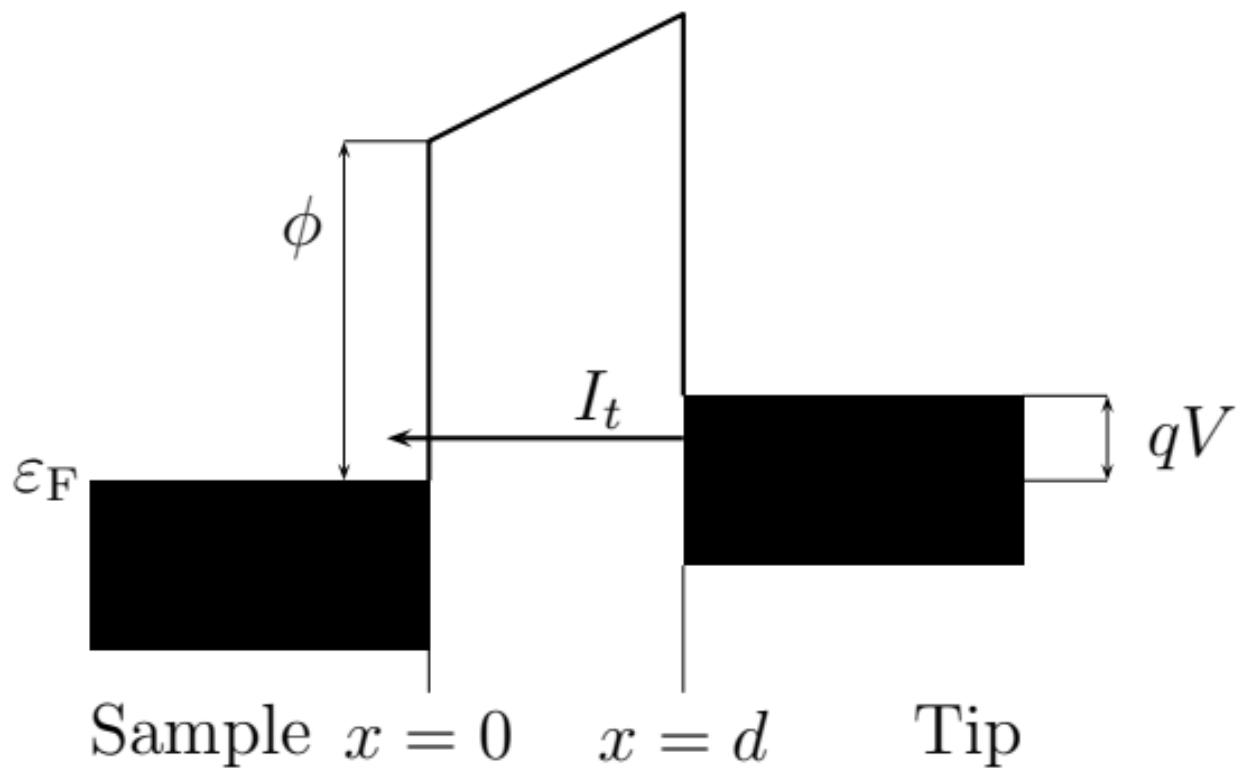
$$I = K \cdot U \cdot \exp(-\kappa \cdot x)$$



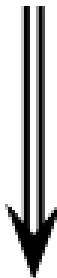
$V_{\text{bias}} < 0$ Vacuum



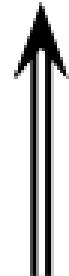
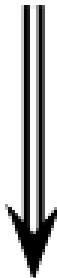
$V_{\text{bias}} > 0$ Vacuum



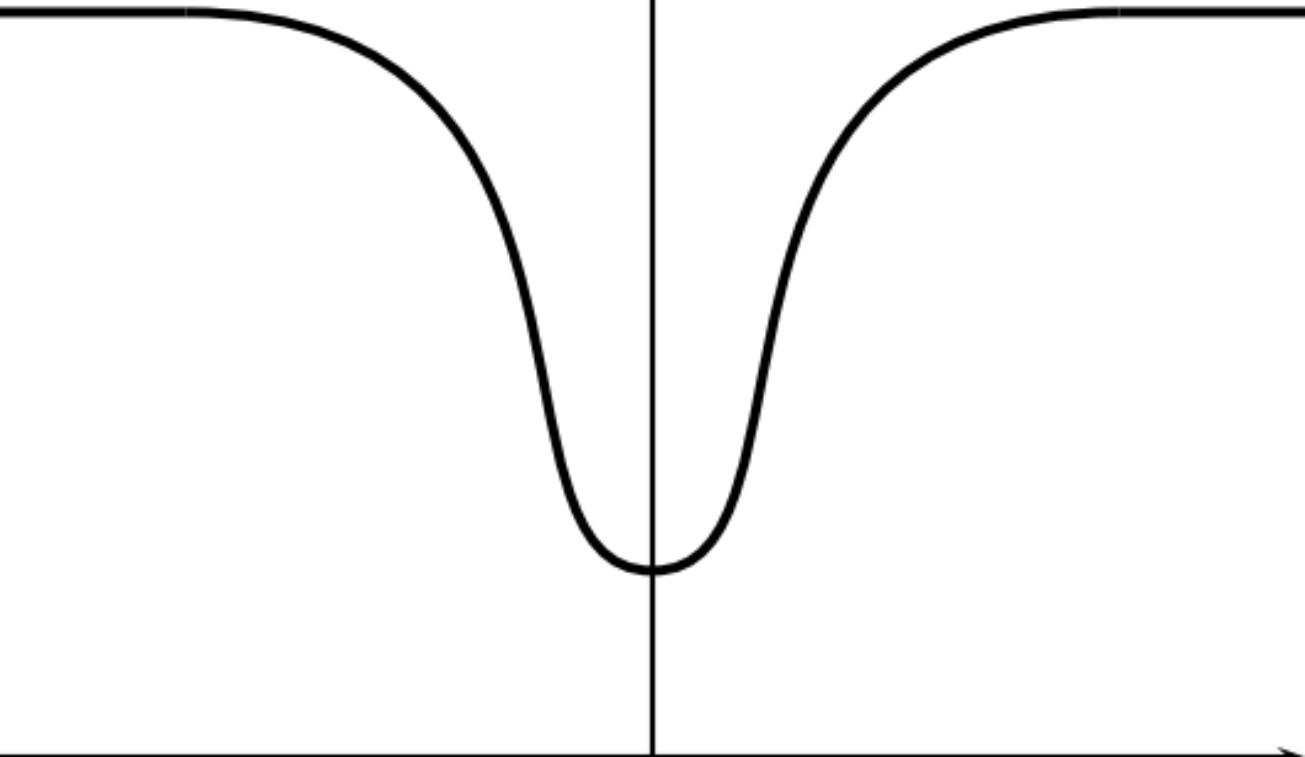
Guess of $n_0(\mathbf{r})$



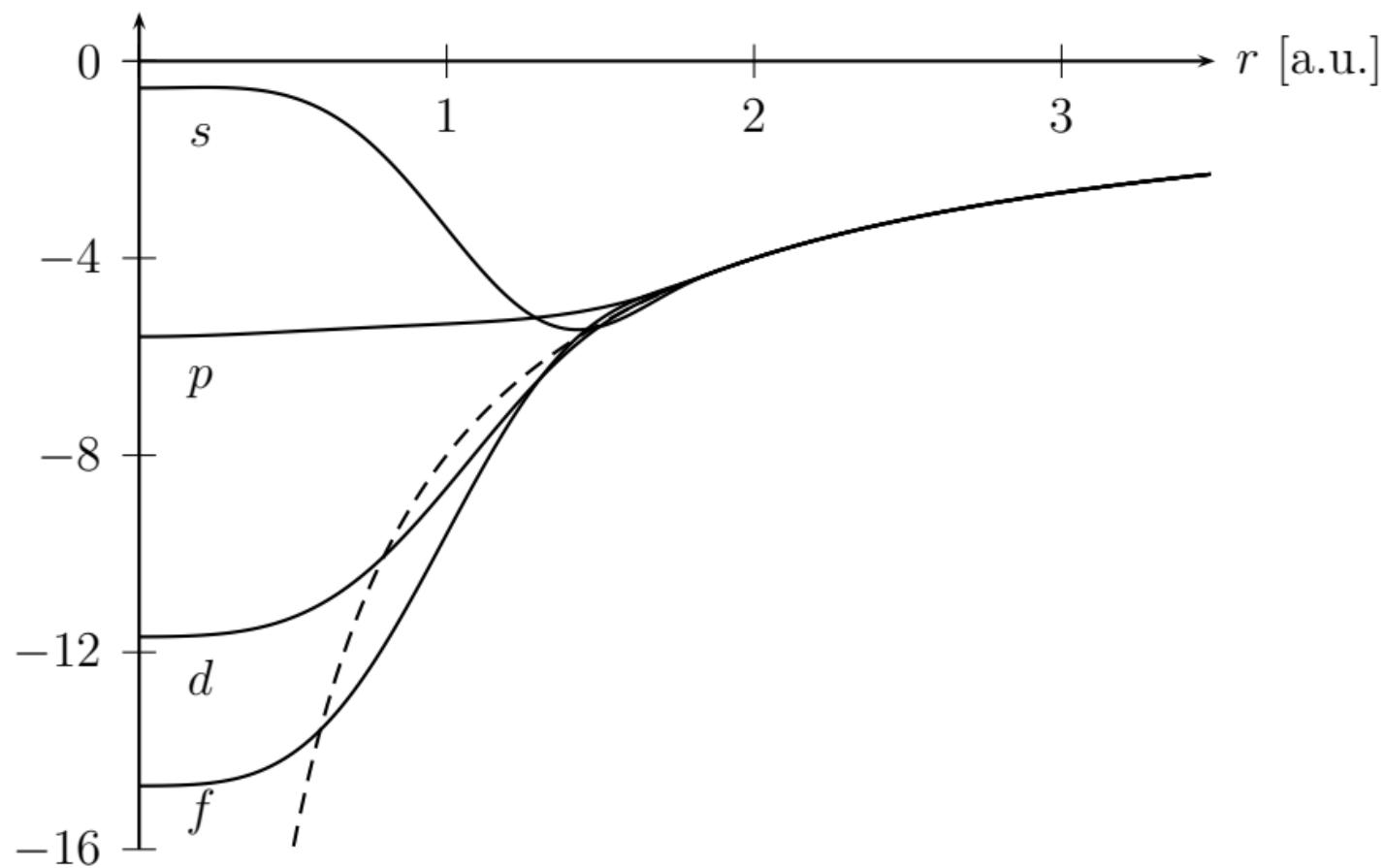
$$V_{\text{ext}}(\mathbf{r}) \longleftrightarrow n_0(\mathbf{r})$$



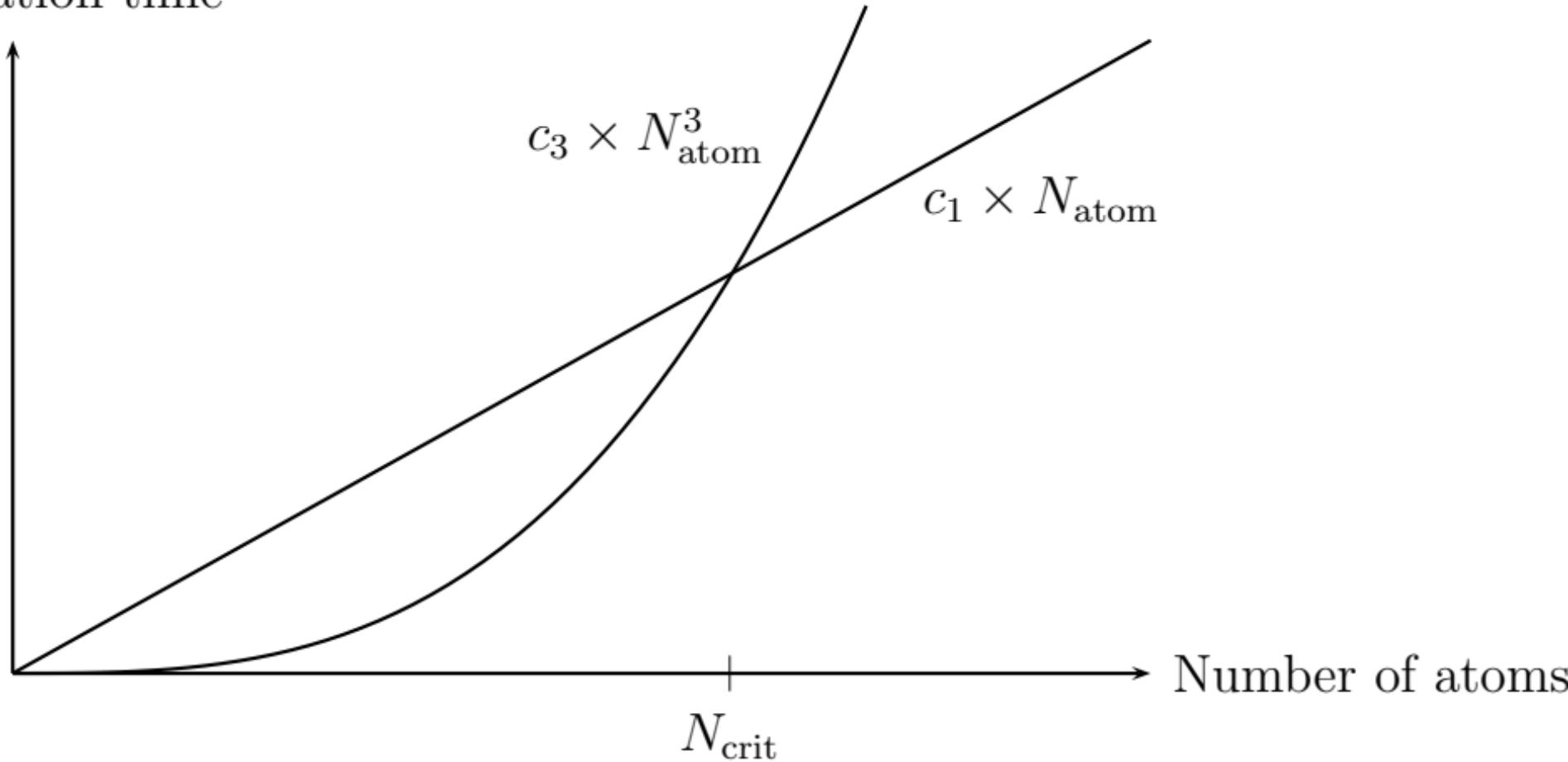
$$\psi_i(\{\mathbf{r}\}) \longrightarrow \psi_0(\{\mathbf{r}\})$$

ρ 

Potential [a.u.]

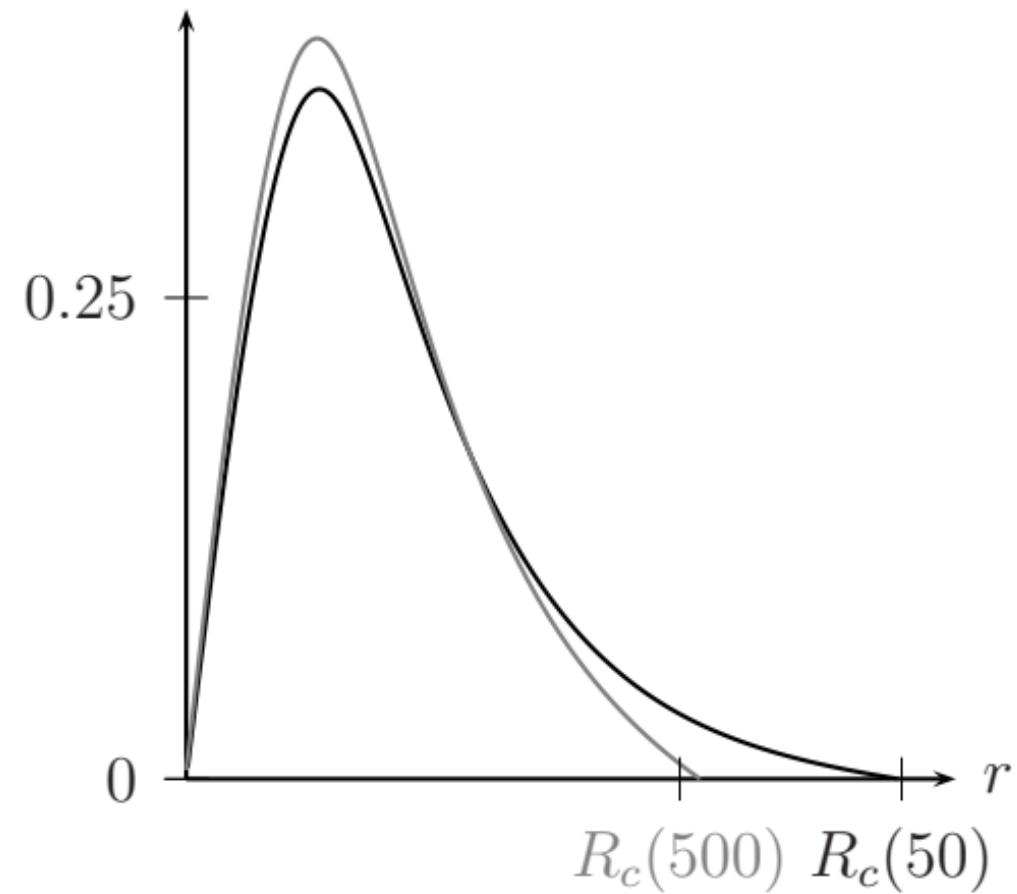
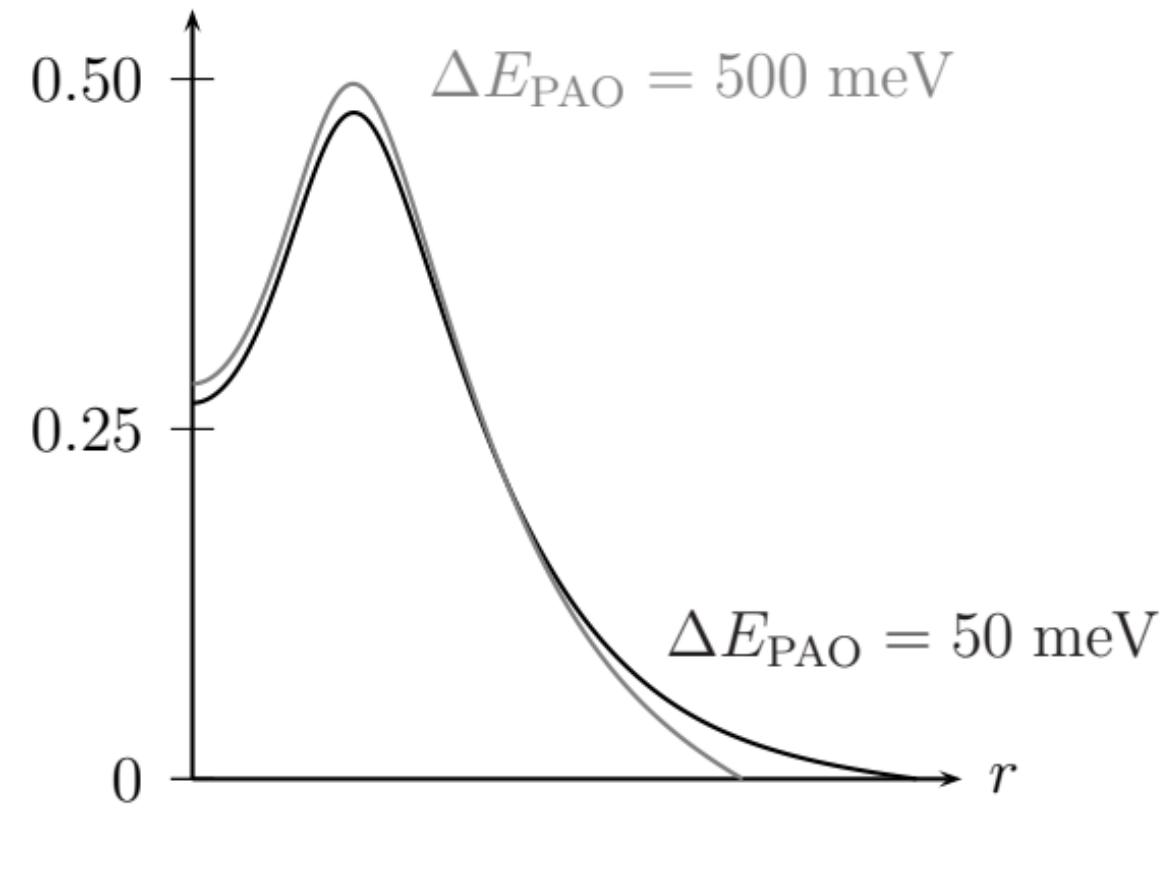


Computation time

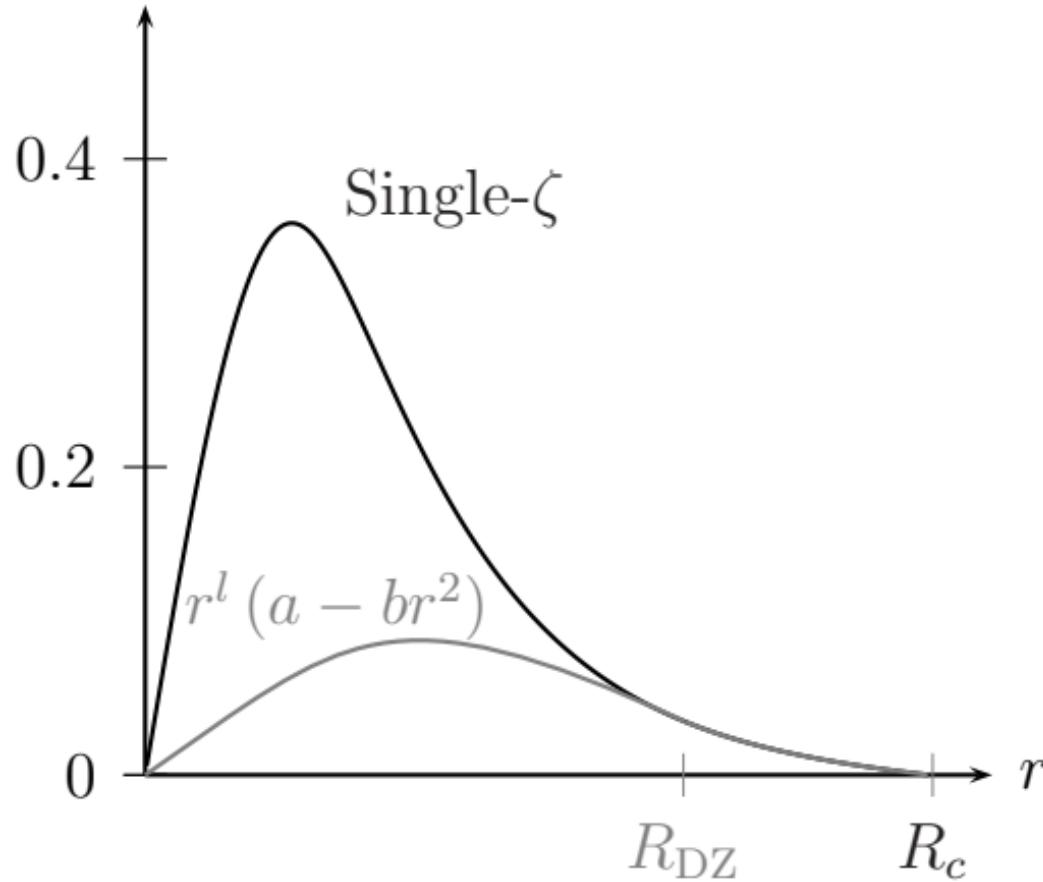


$\phi(r)$, s-orbital

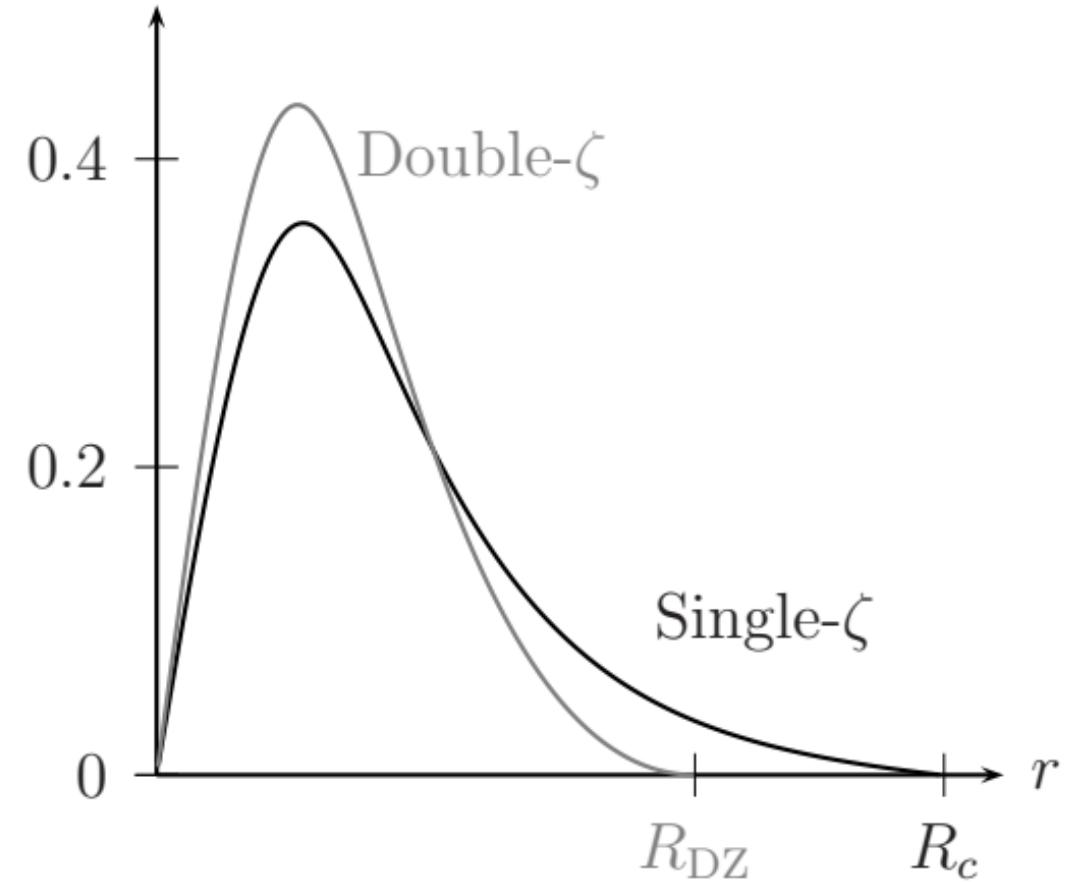
$\phi(r)$, p-orbital

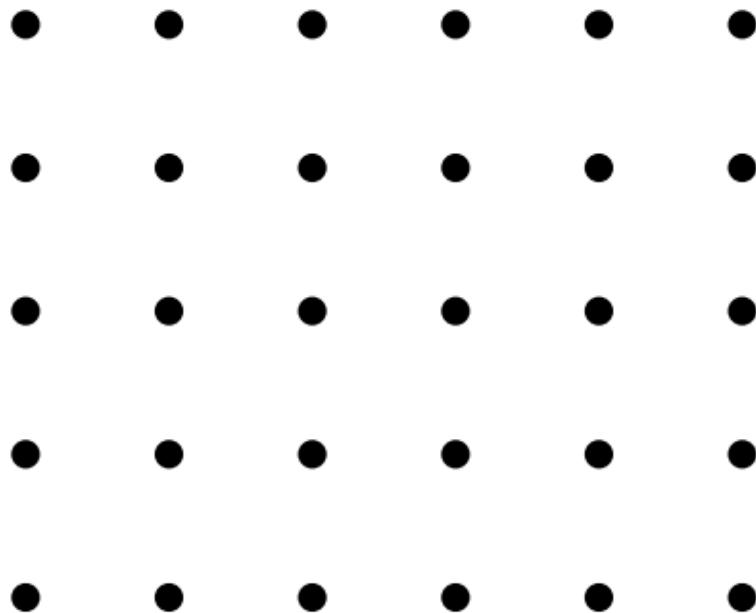


$\phi(r)$, p-orbital



$\phi(r)$, p-orbital

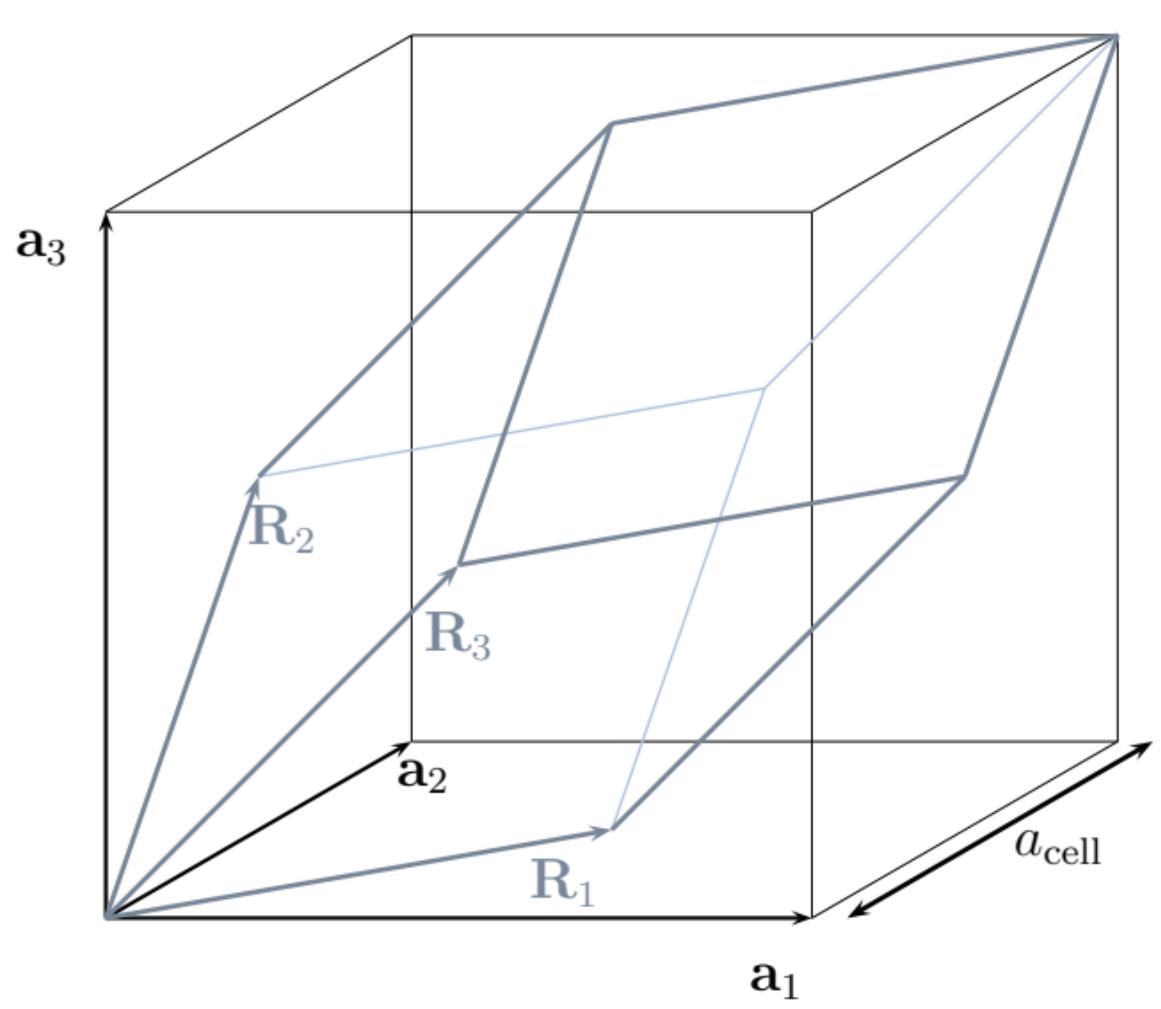


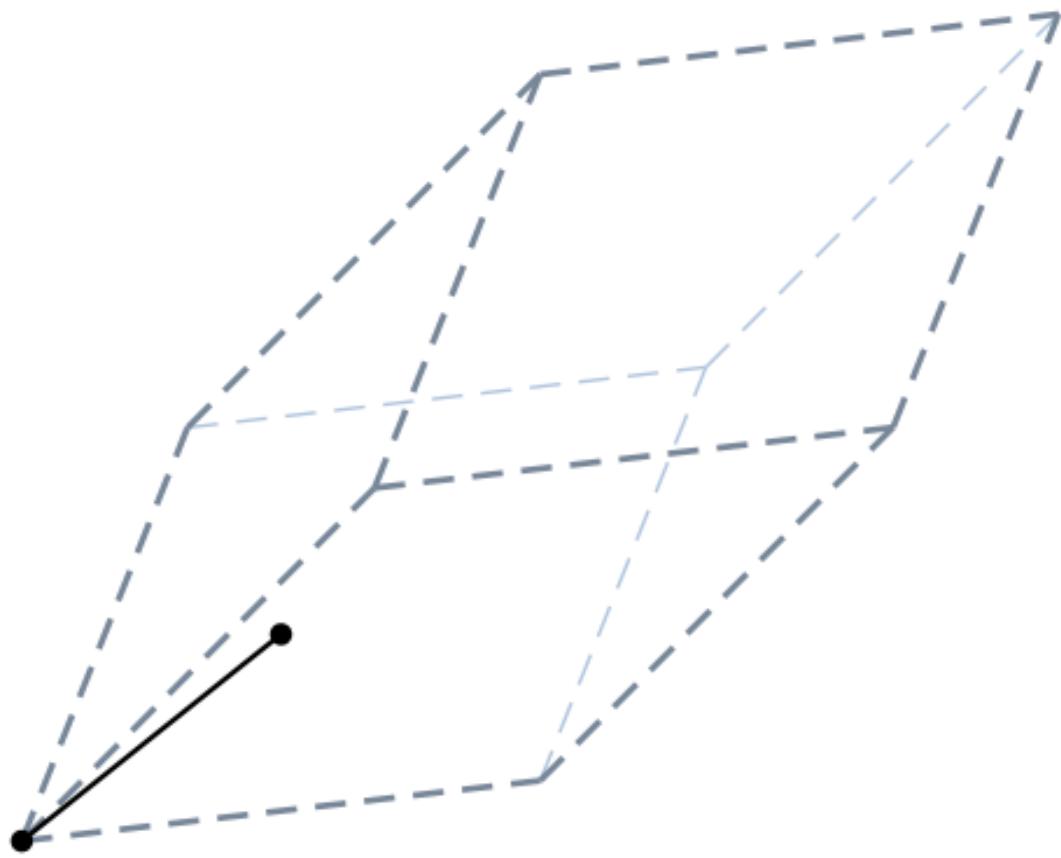


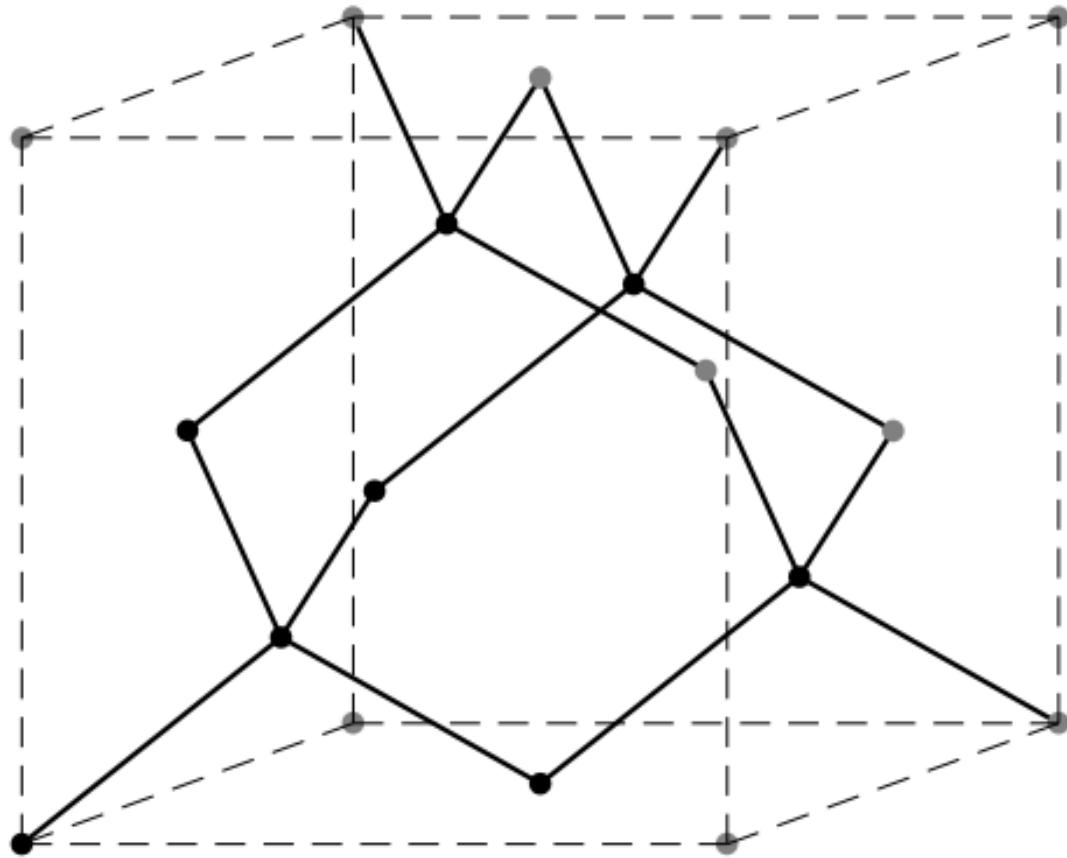
$$k_c = \frac{\pi}{\Delta x}$$

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

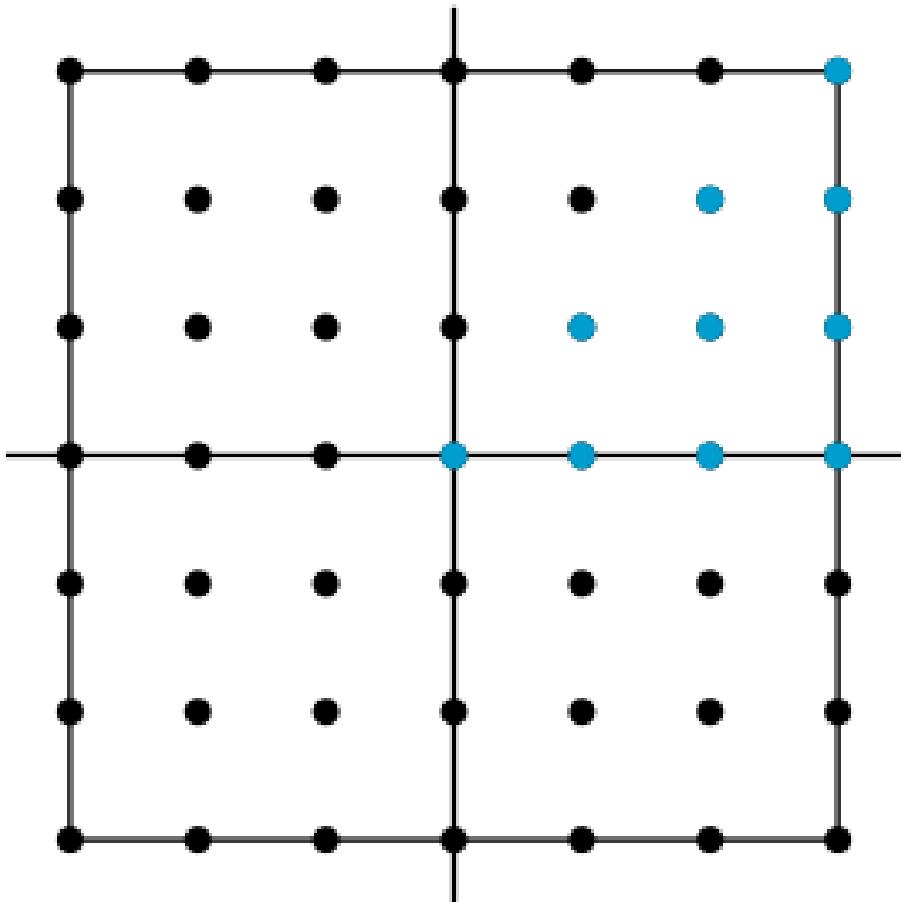




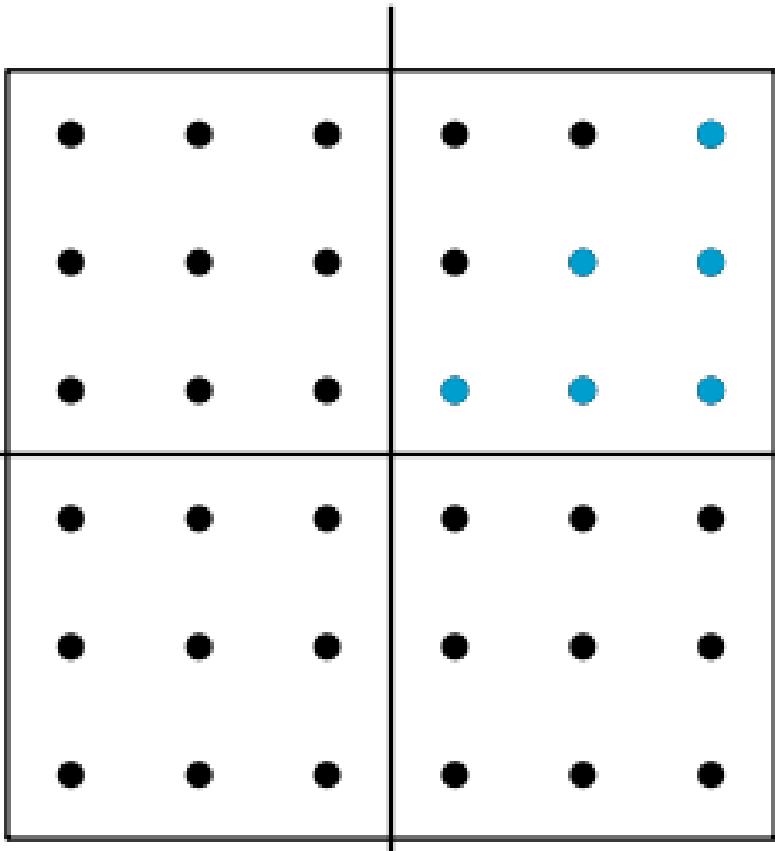




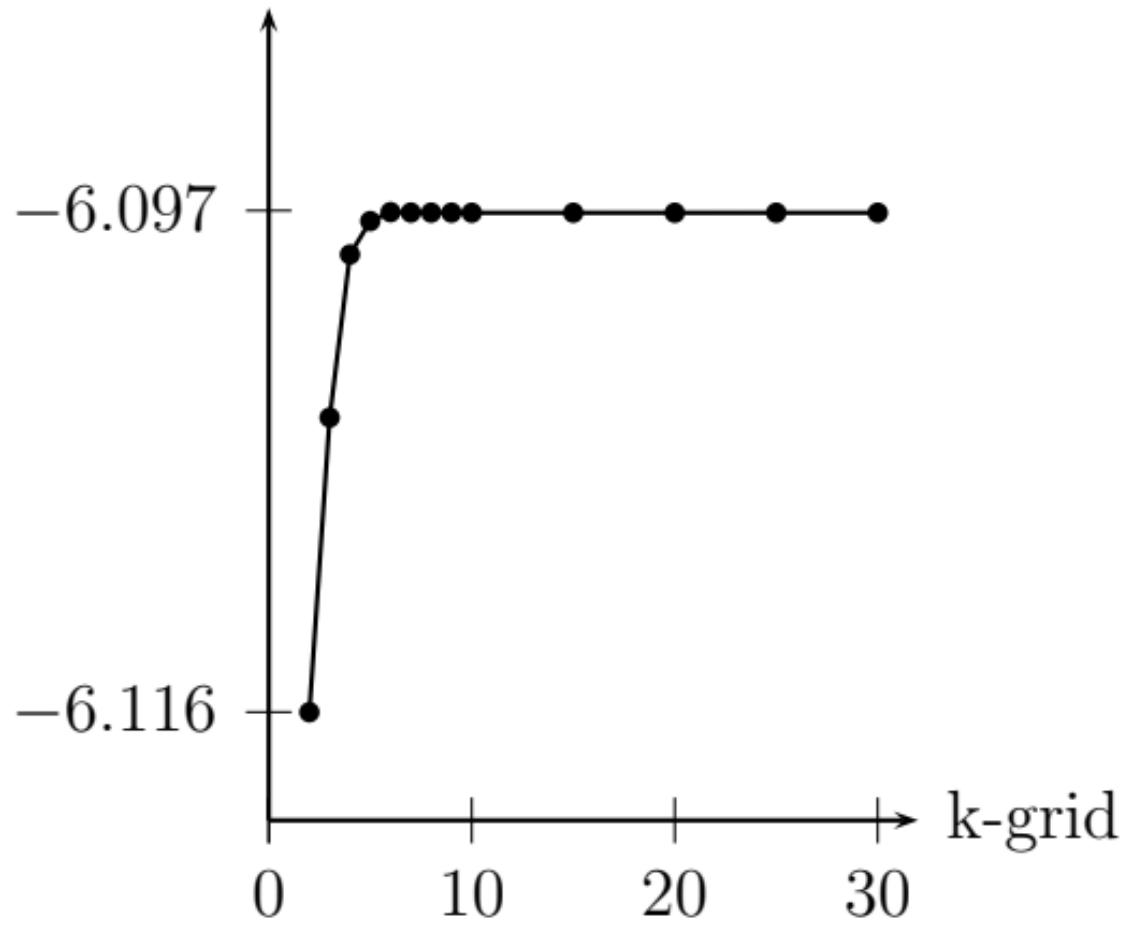
Regular Grid

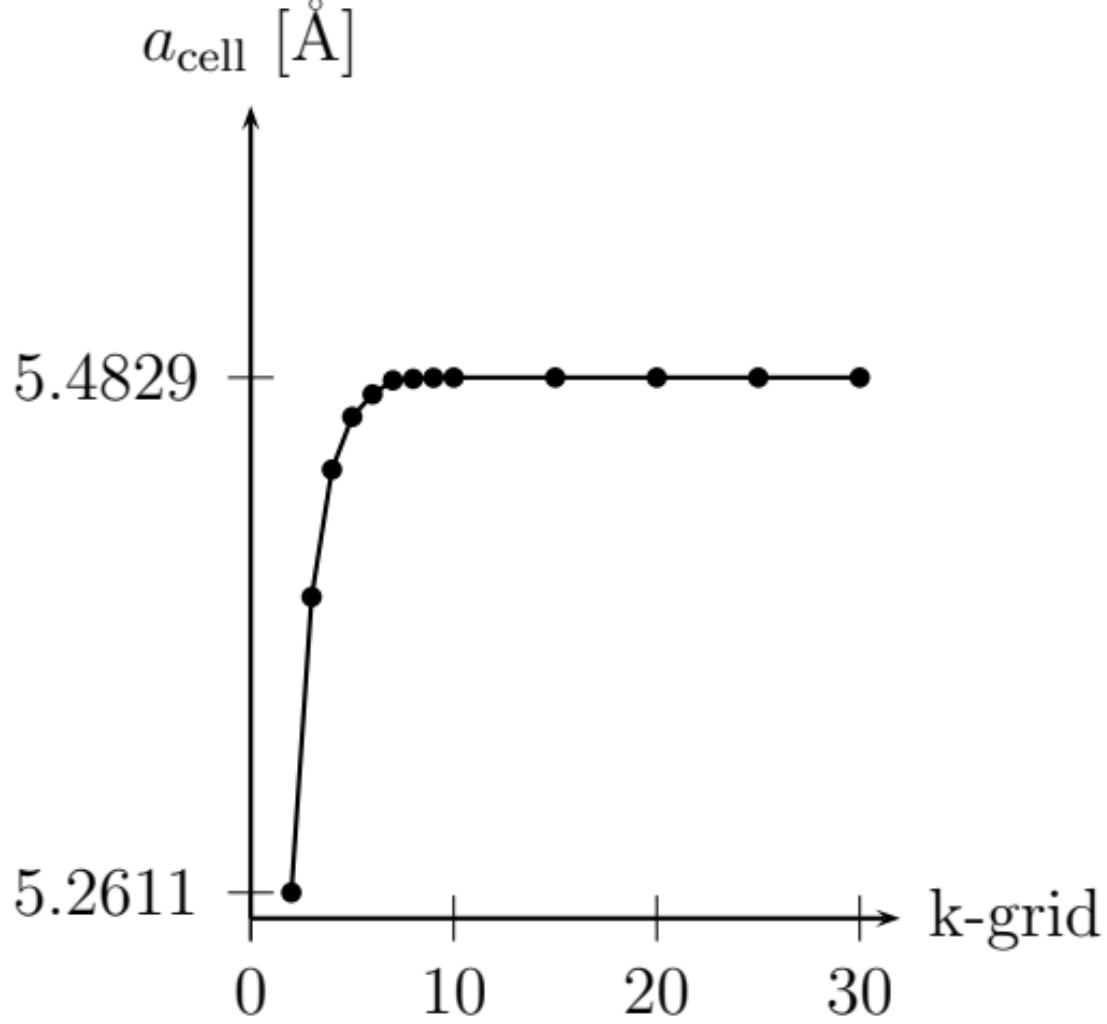


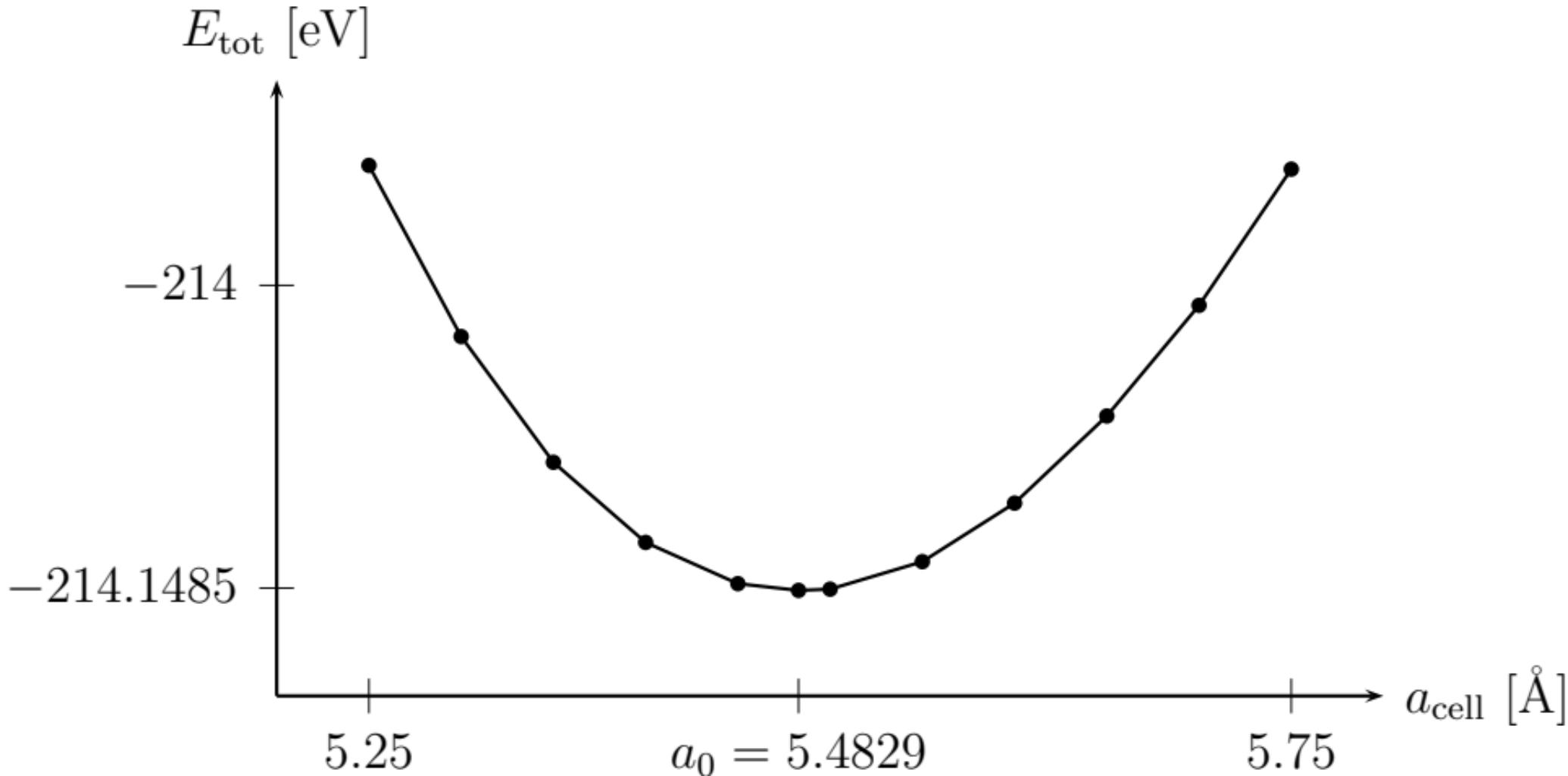
Shifted Grid

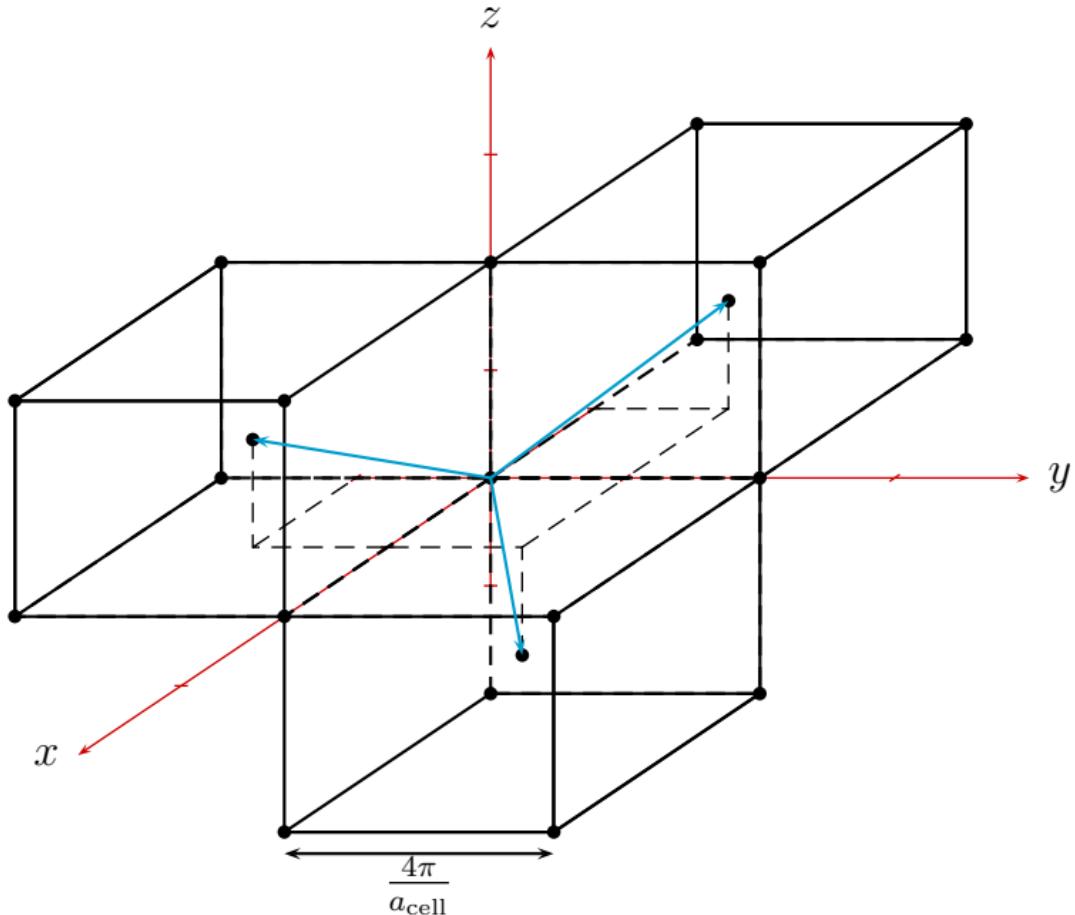


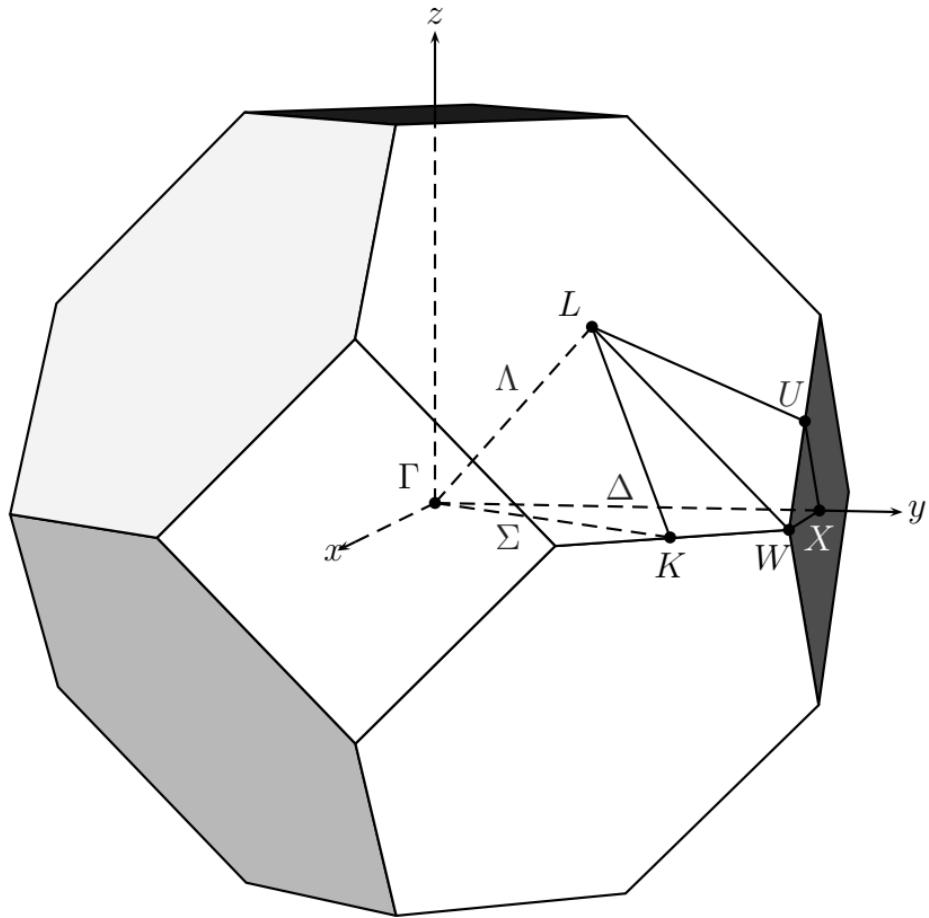
Cohesion Energy [eV]

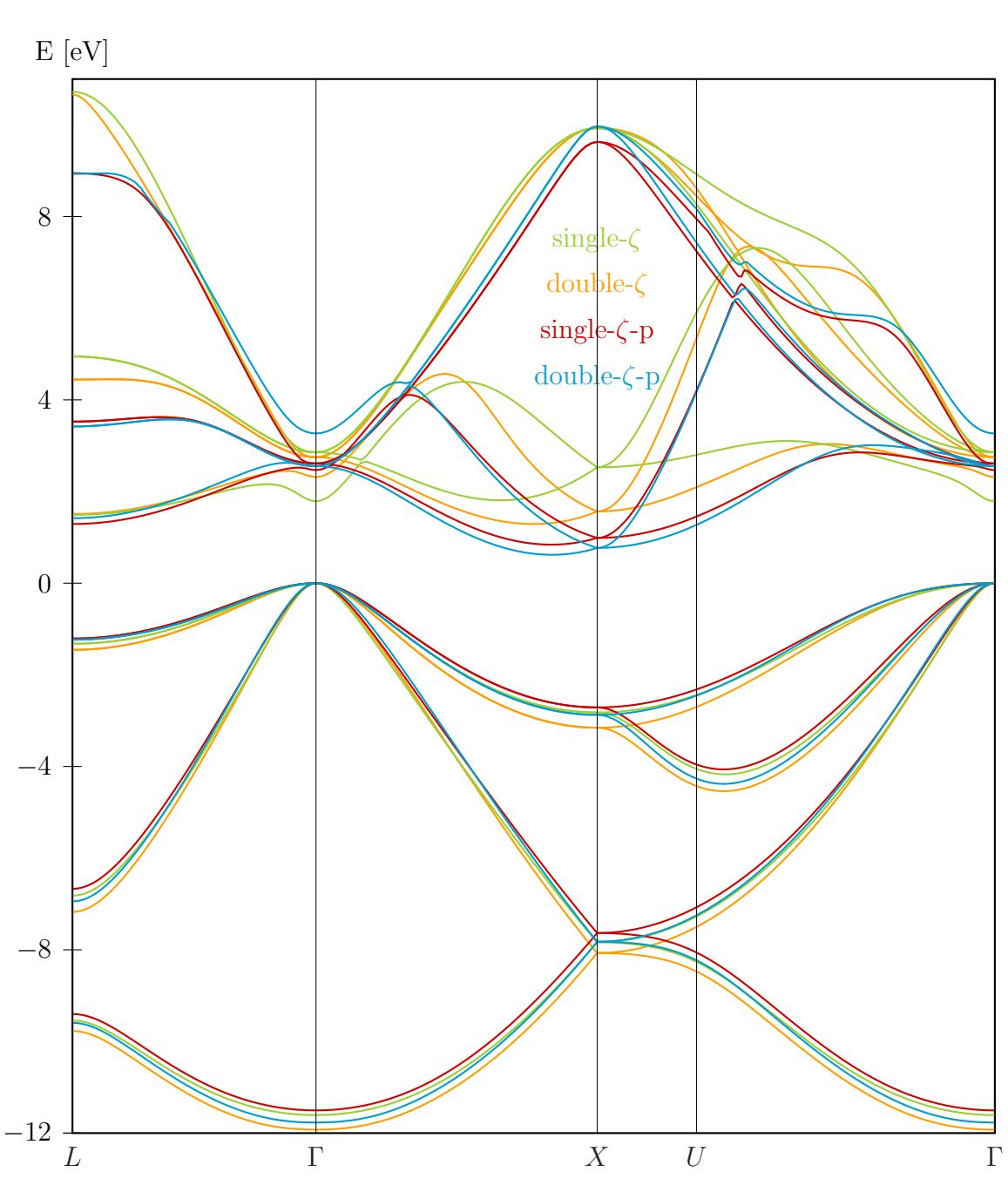


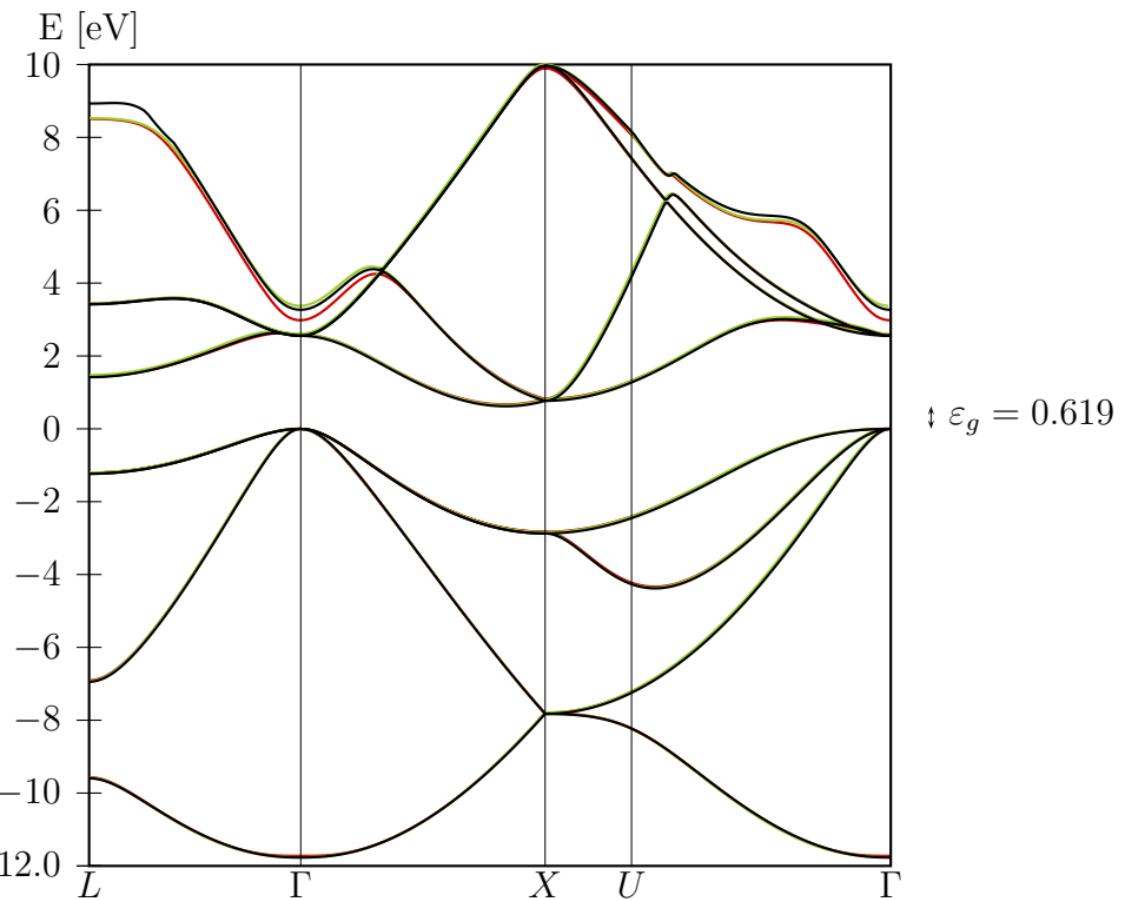


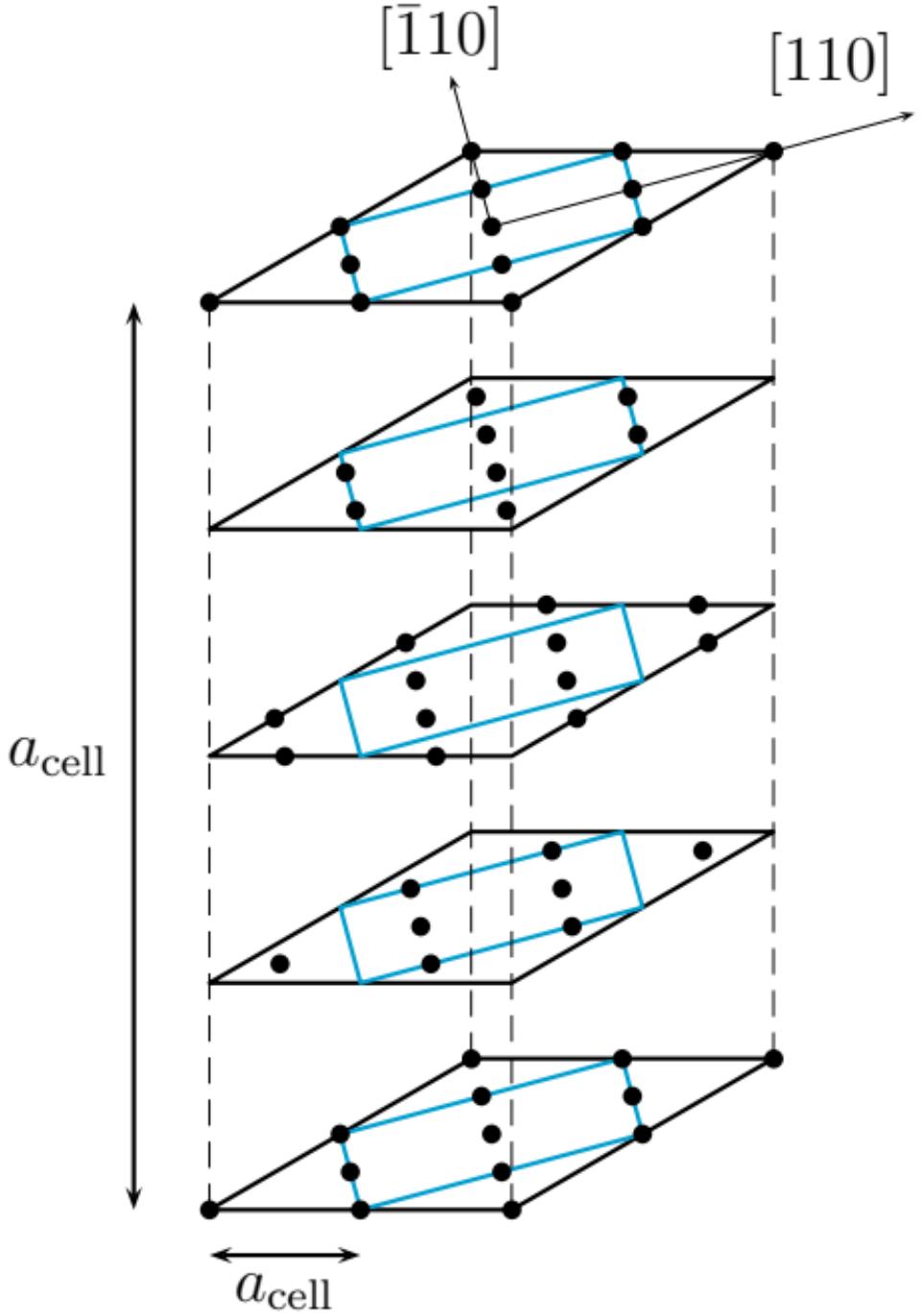


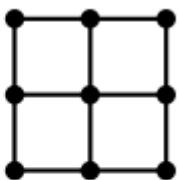




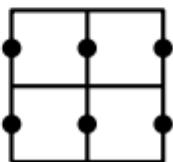






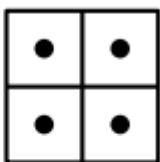


$$z = a_{\text{cell}}$$

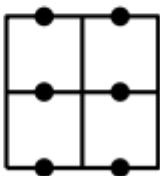


$$z = 0.75 \cdot a_{\text{cell}}$$

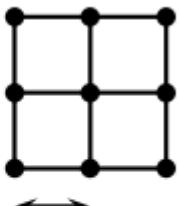
[$\bar{1}10$]



$$z = 0.5 \cdot a_{\text{cell}}$$



$$z = 0.25 \cdot a_{\text{cell}}$$

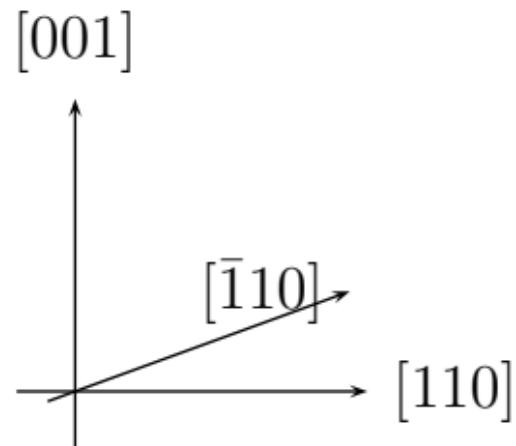
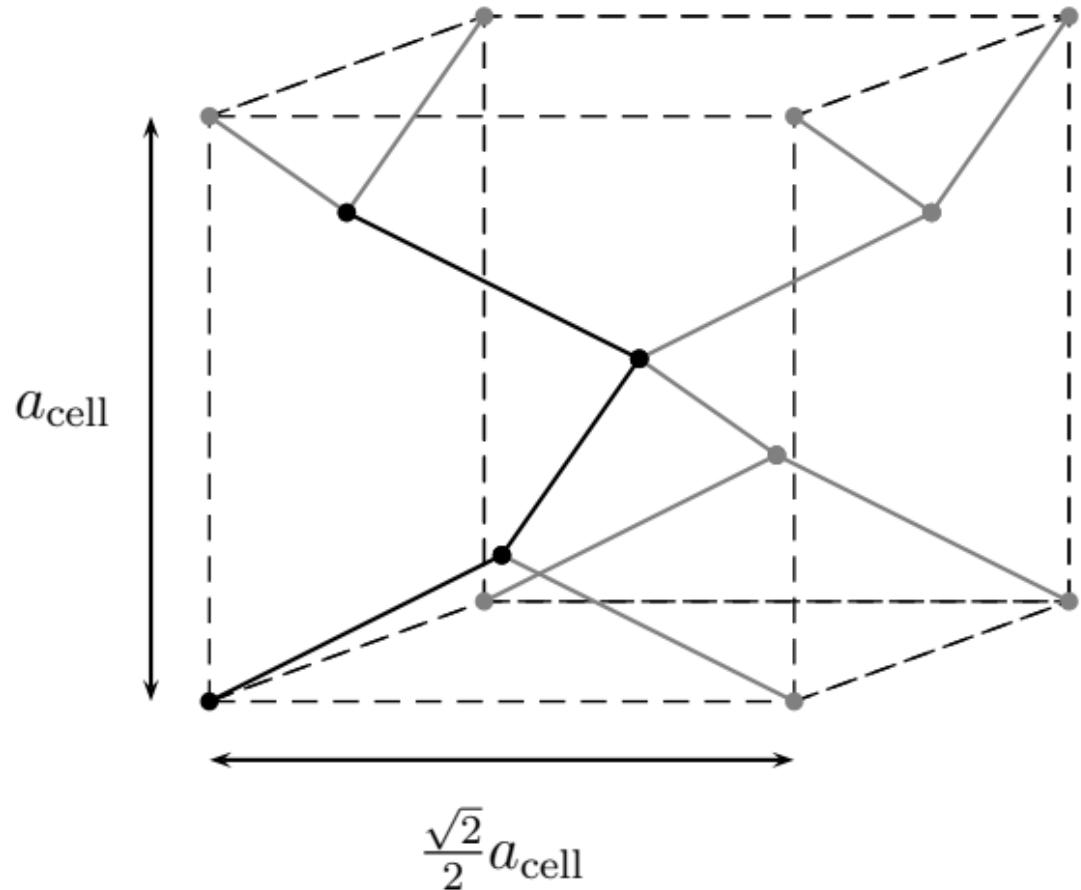


$$z = 0$$

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



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





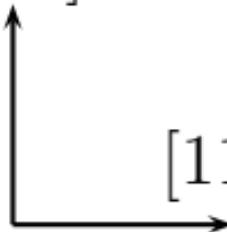
Adding free volume

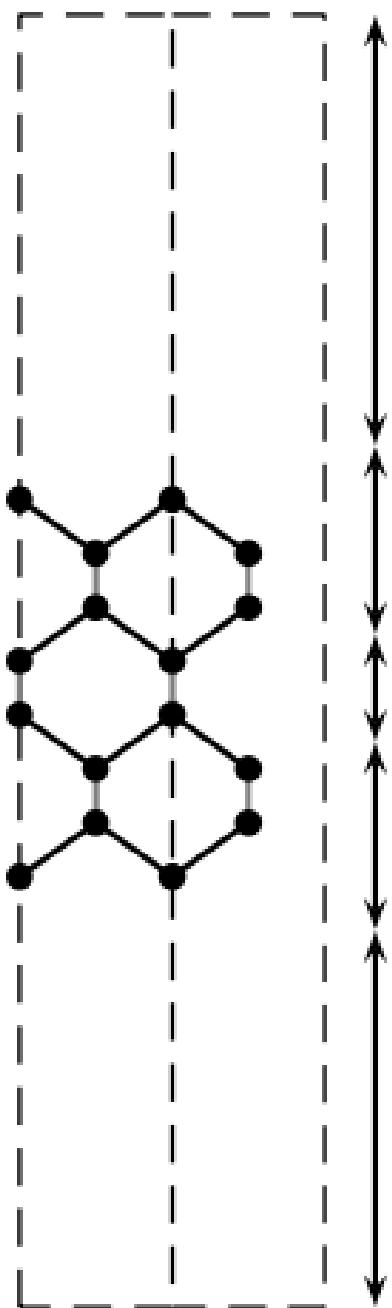


[001]



[110]





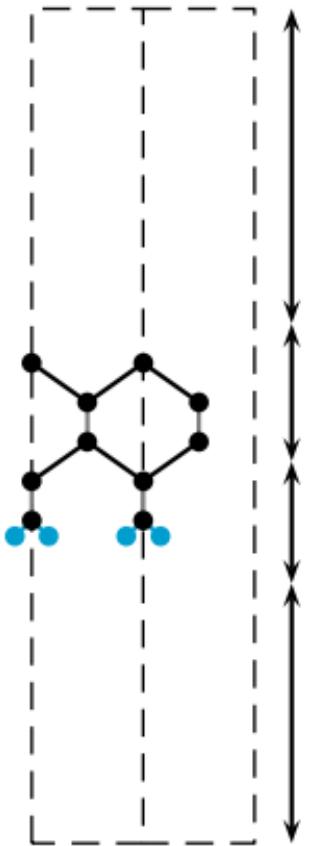
Free volume

Relaxed

Fixed

Relaxed

Free volume



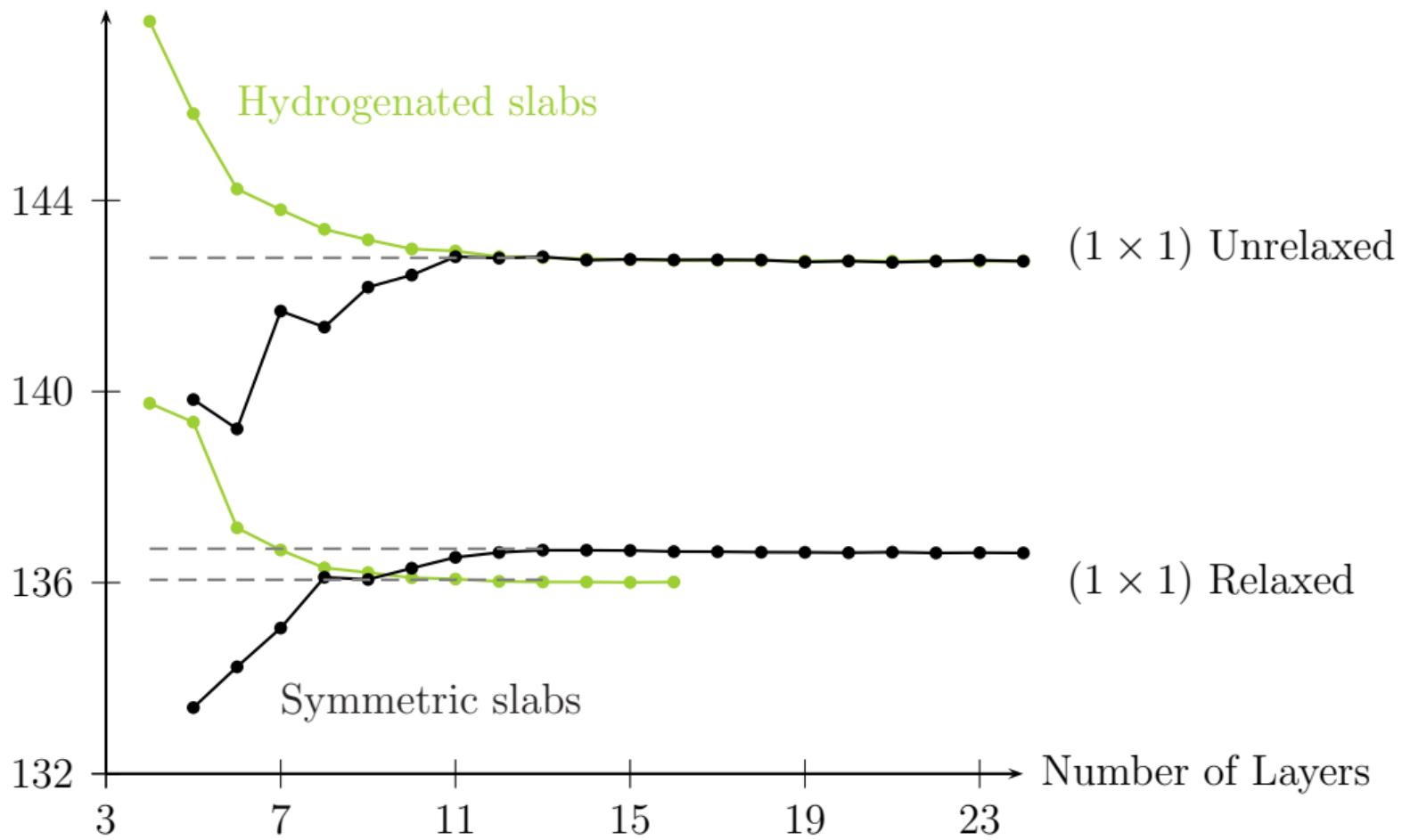
Free volume

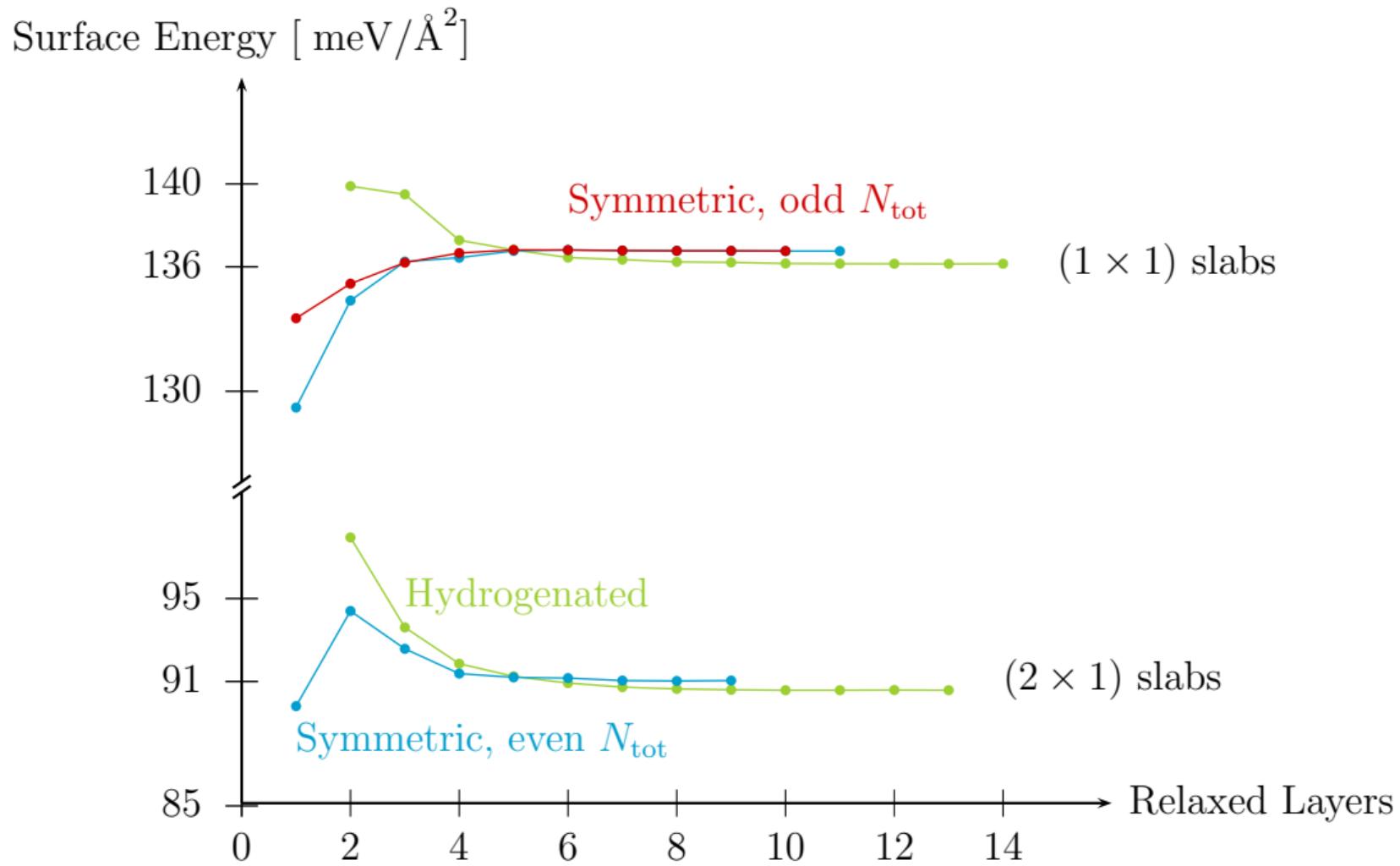
Relaxed

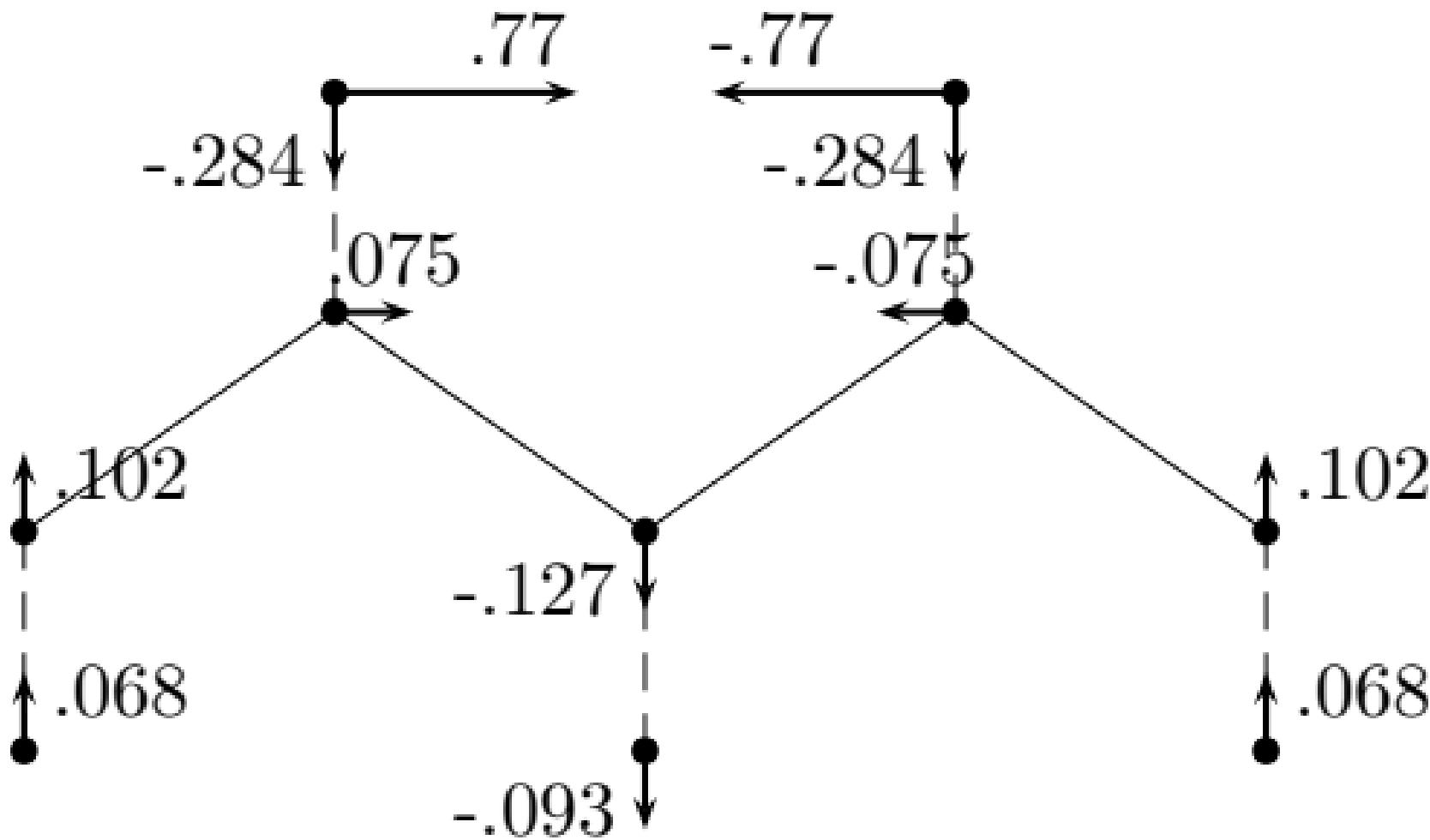
Fixed, with hydrogens

Free volume

Surface Energy [meV/ \AA^2]







2.336

2.334

2.383

2.374

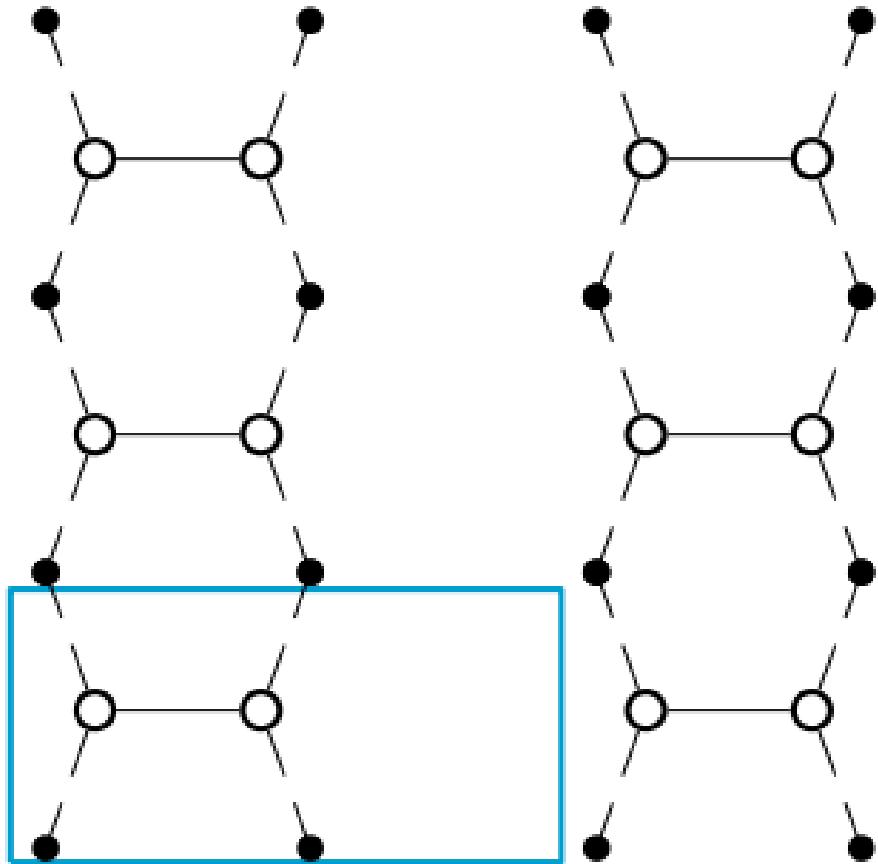
2.334

2.374

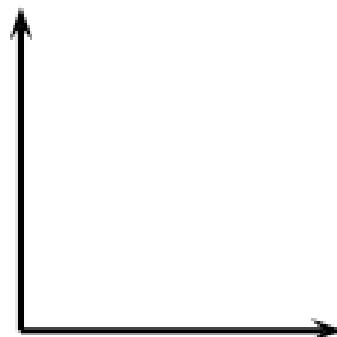
2.355

2.394

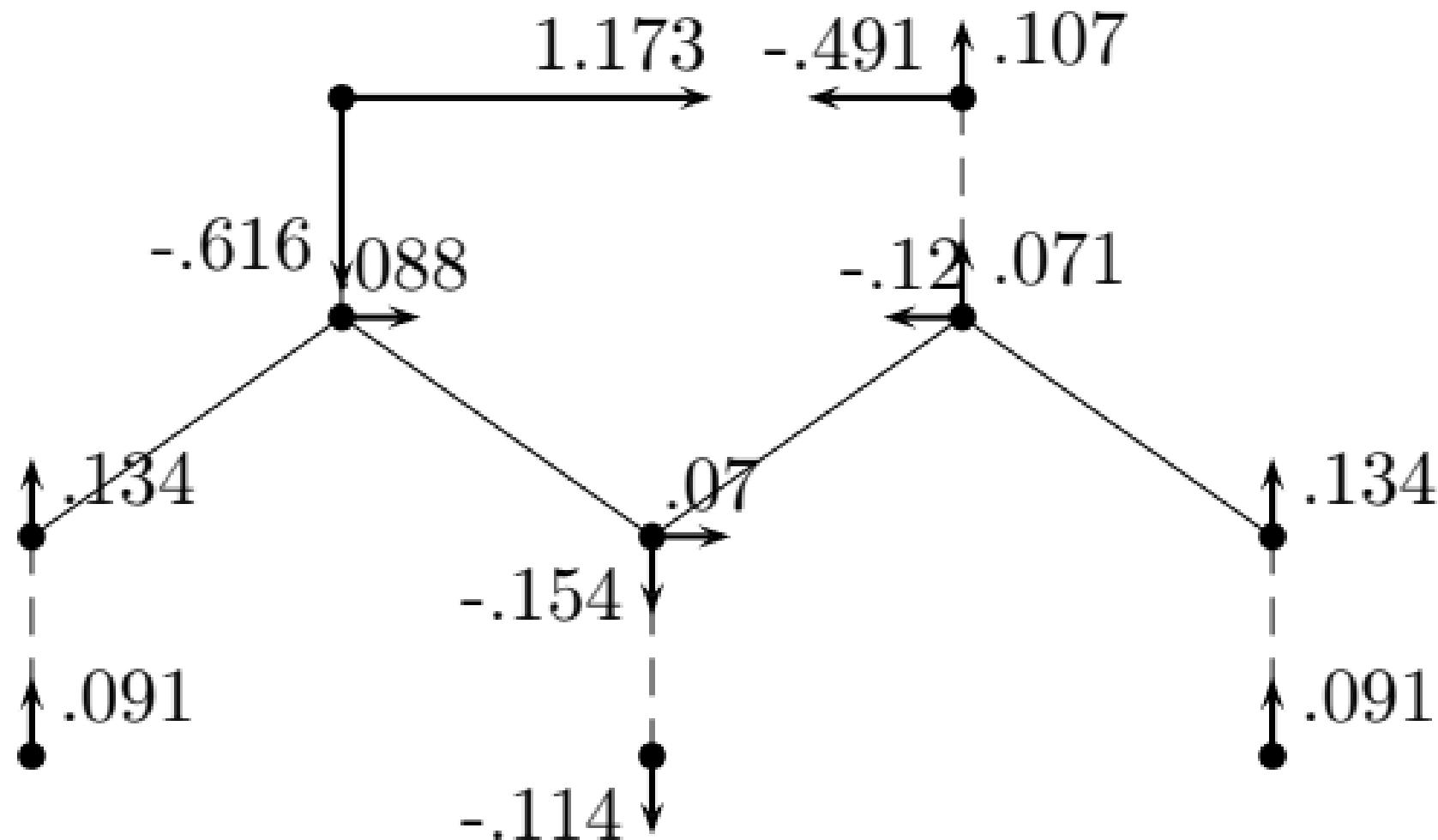
2.394

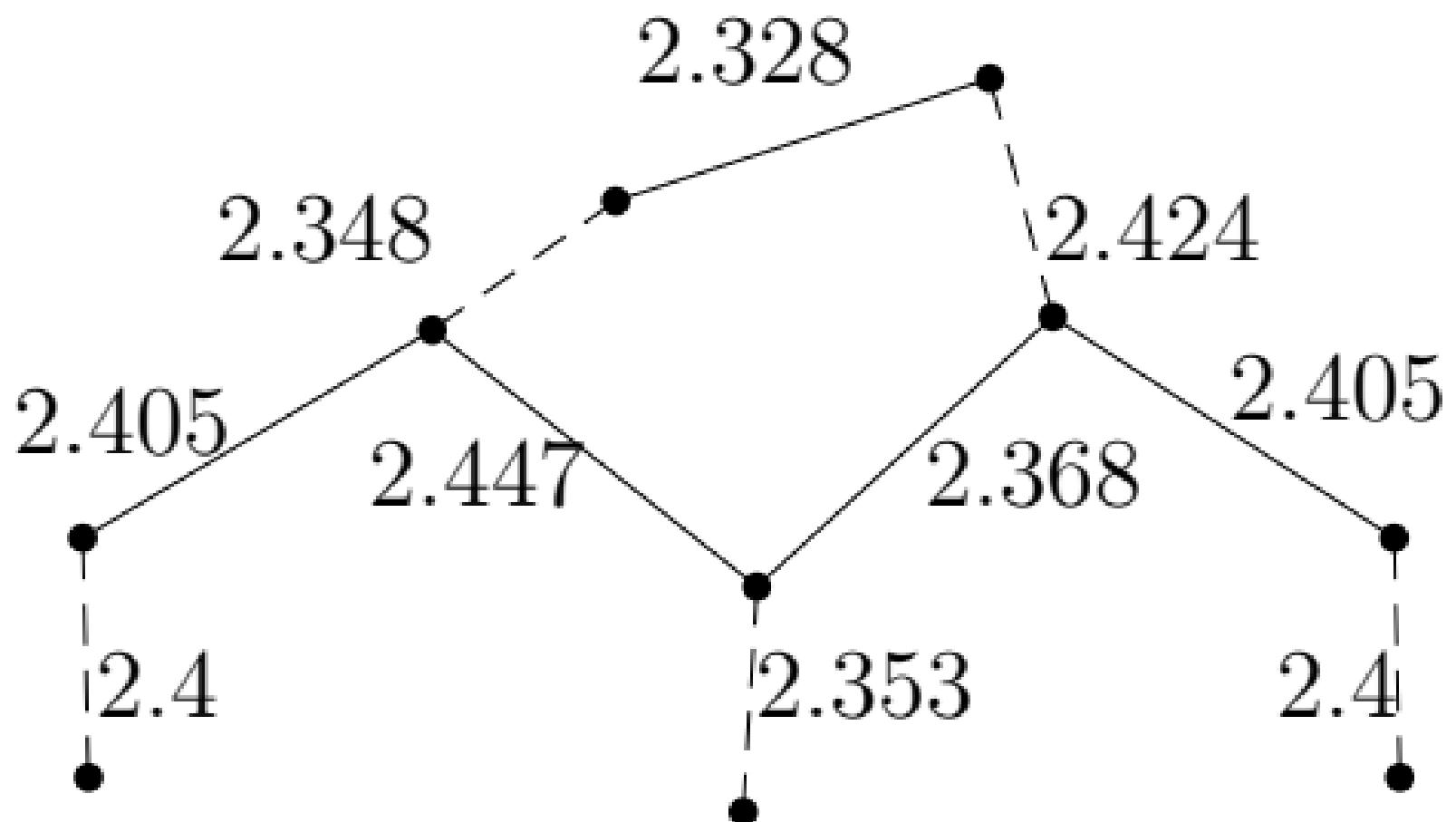


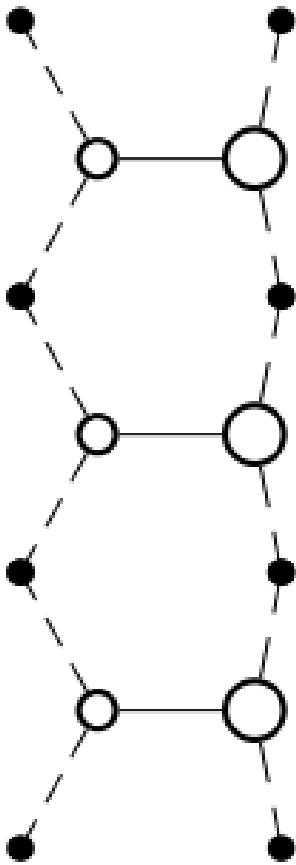
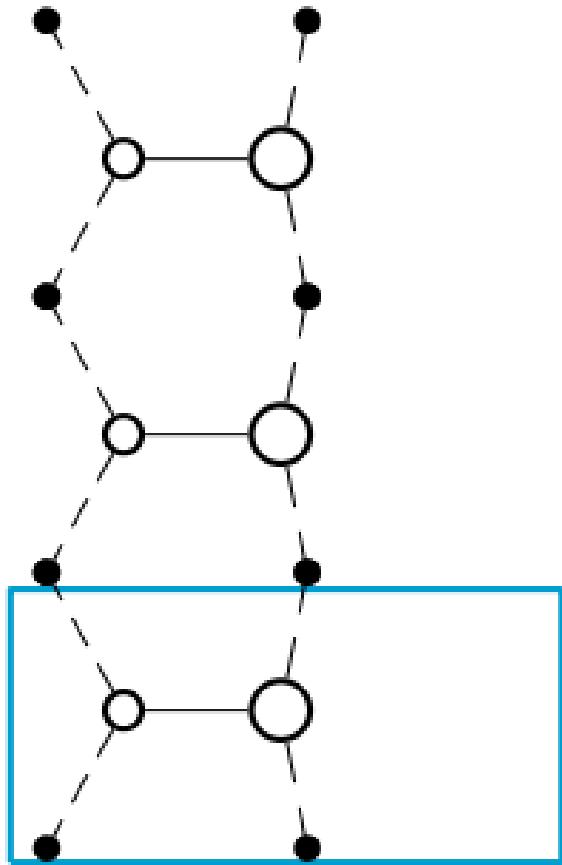
$[\bar{1}10]$



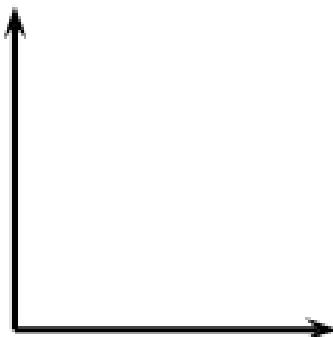
$[110]$



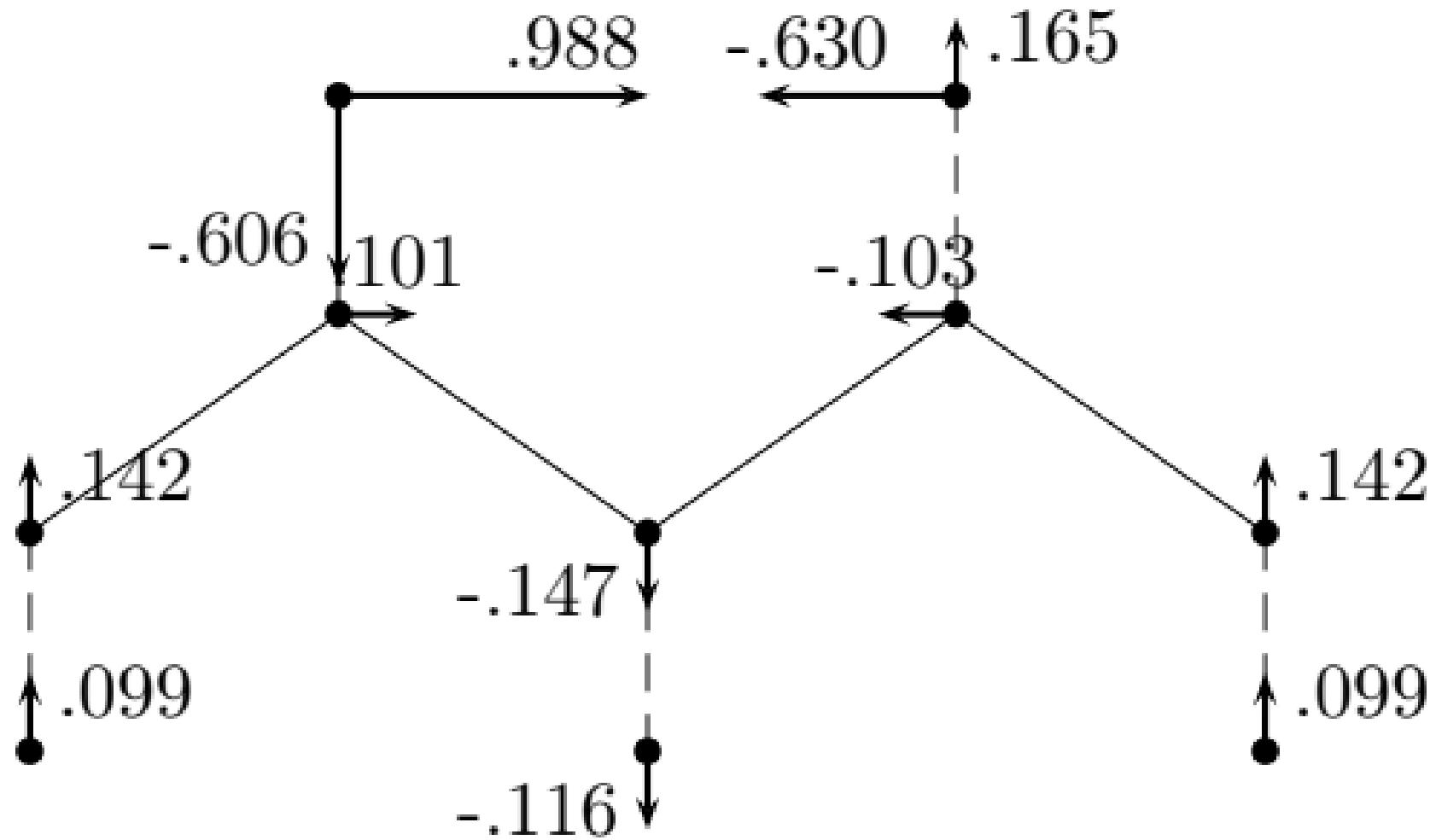


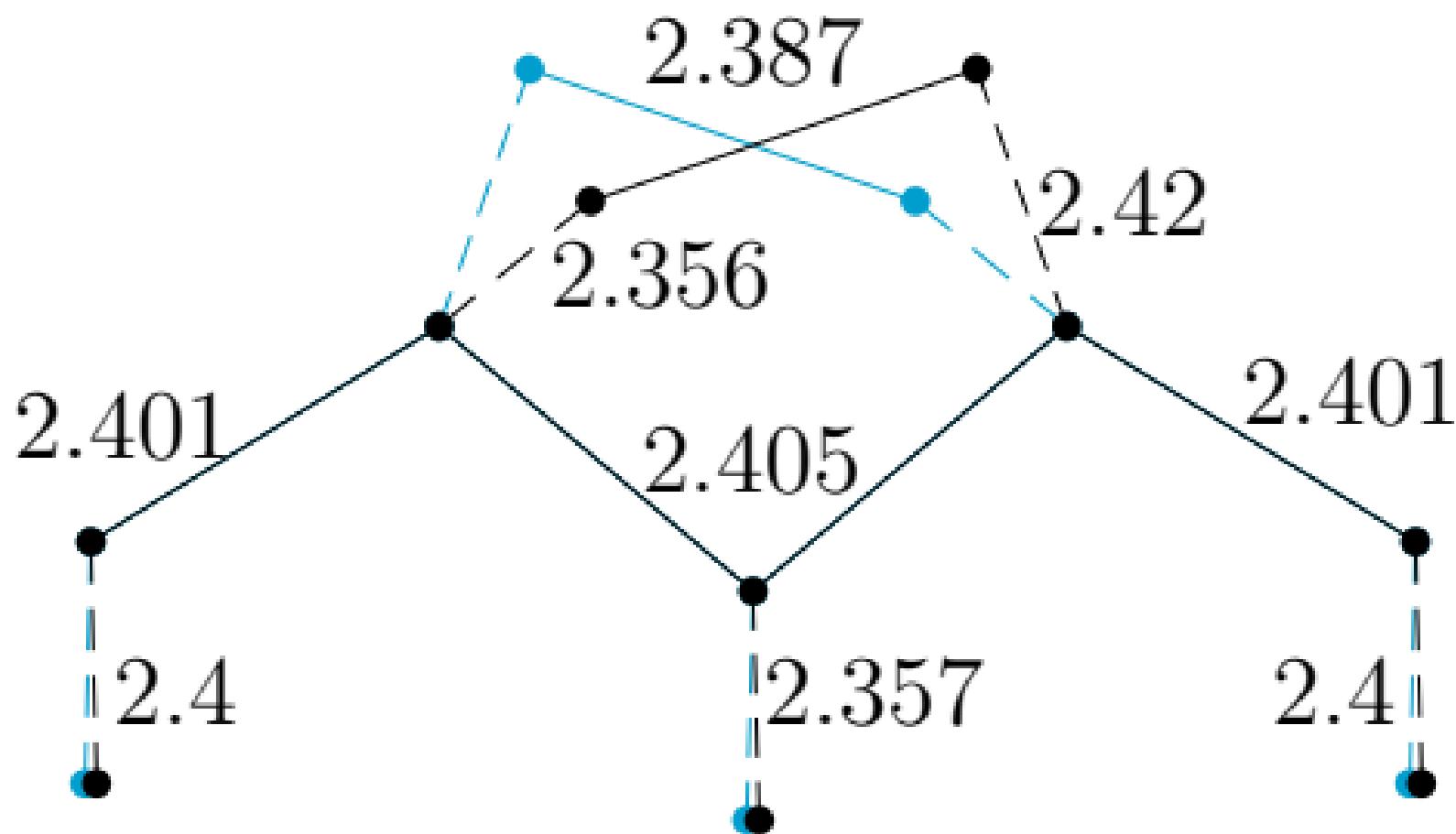


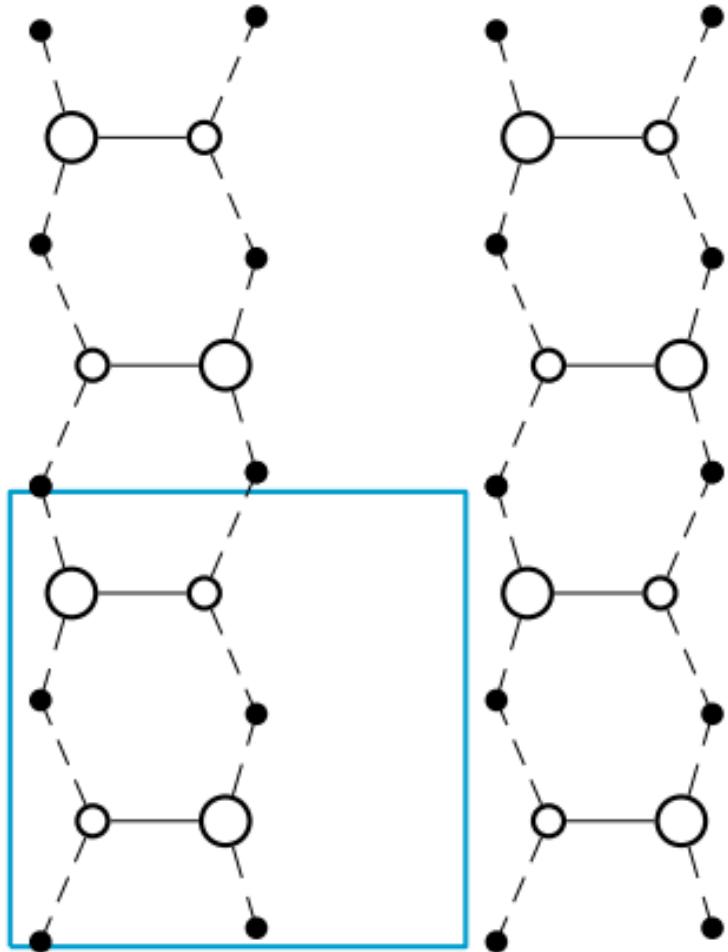
$[\bar{1}10]$



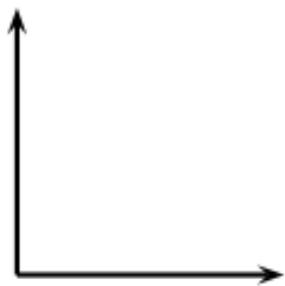
$[110]$



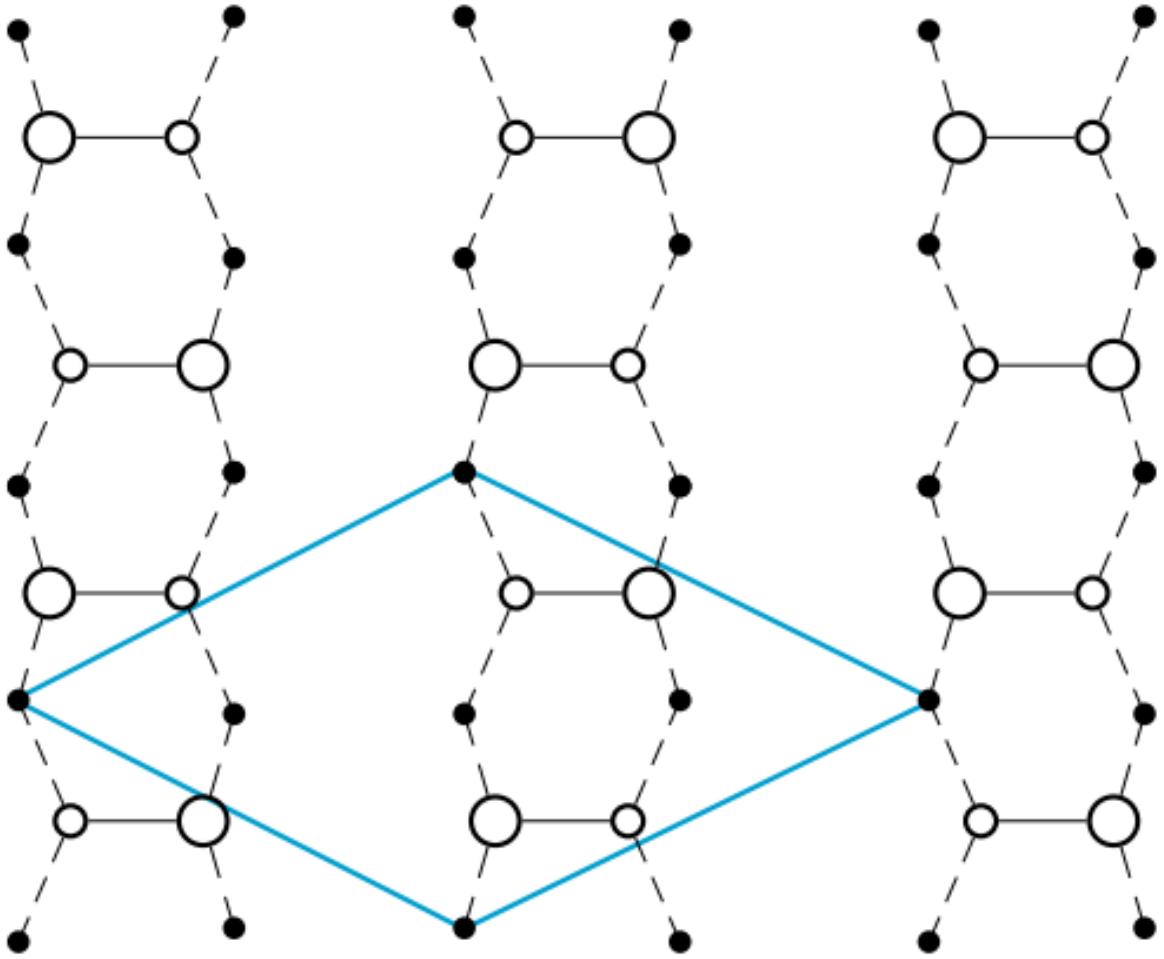




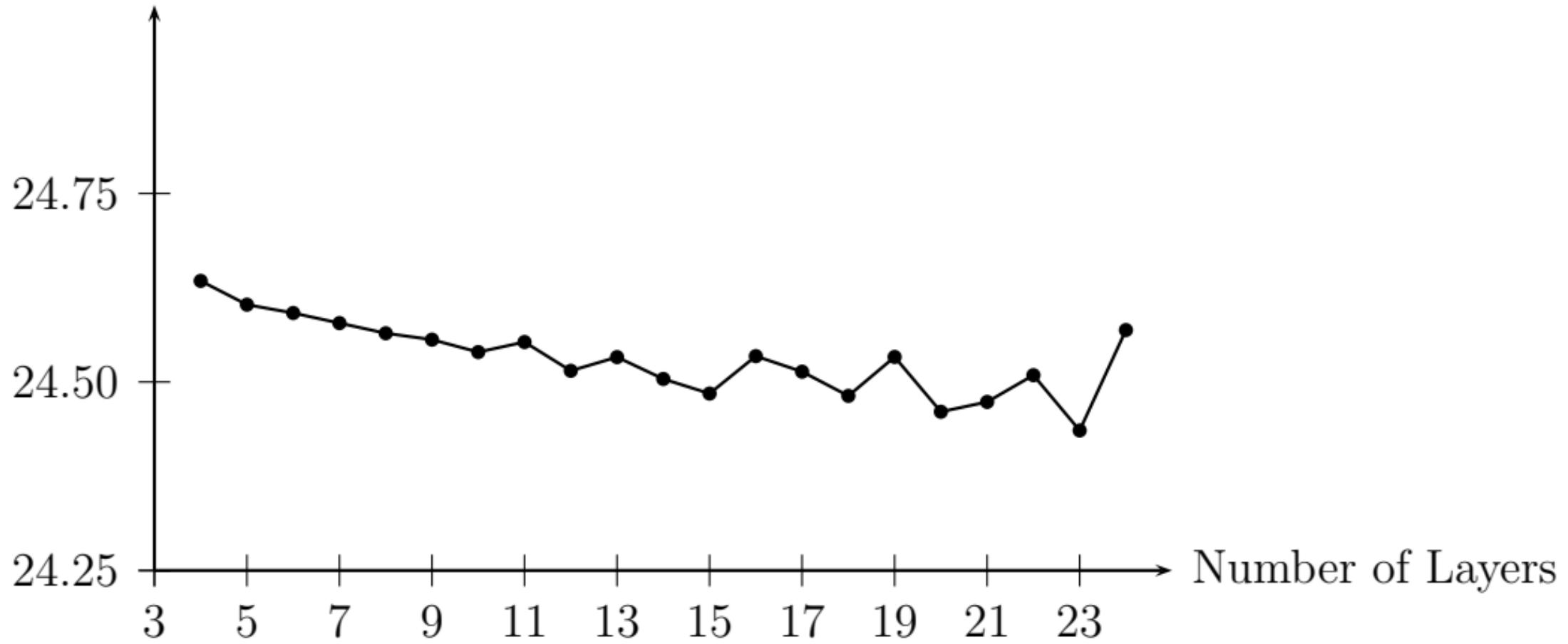
$[\bar{1}10]$



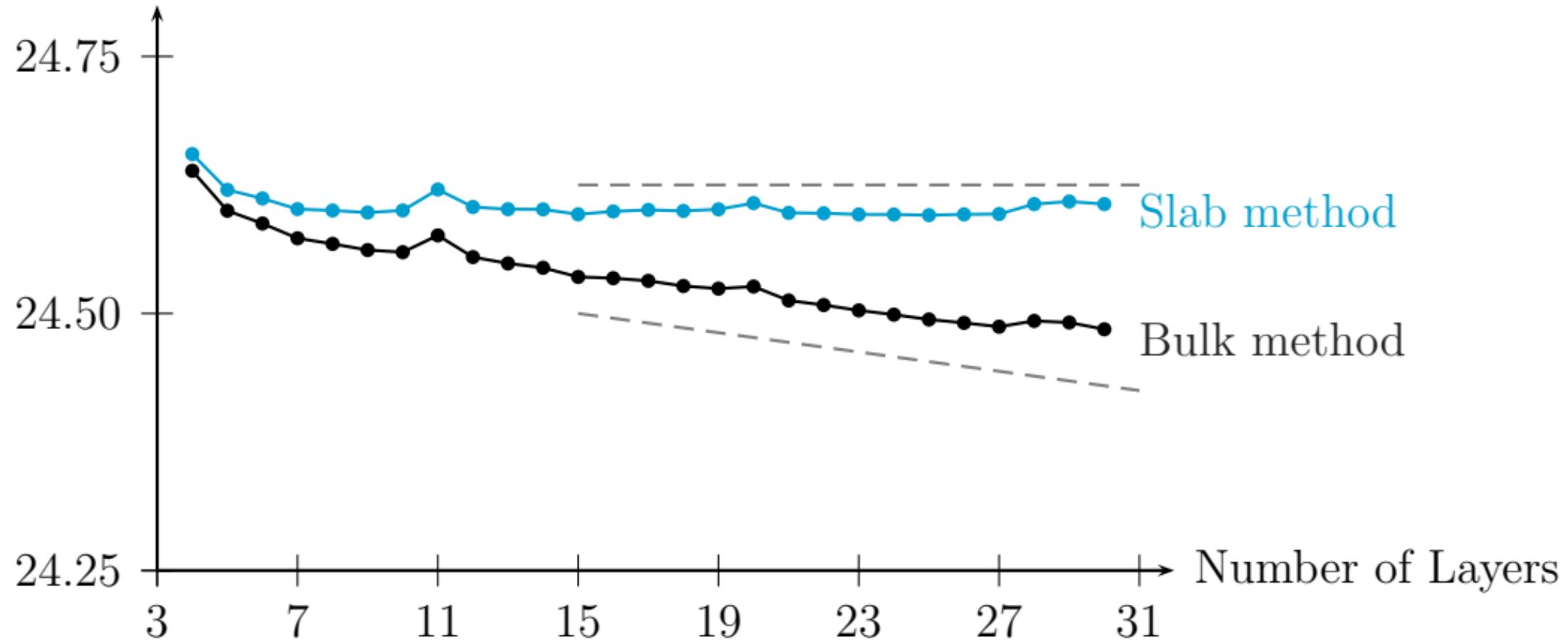
$[110]$



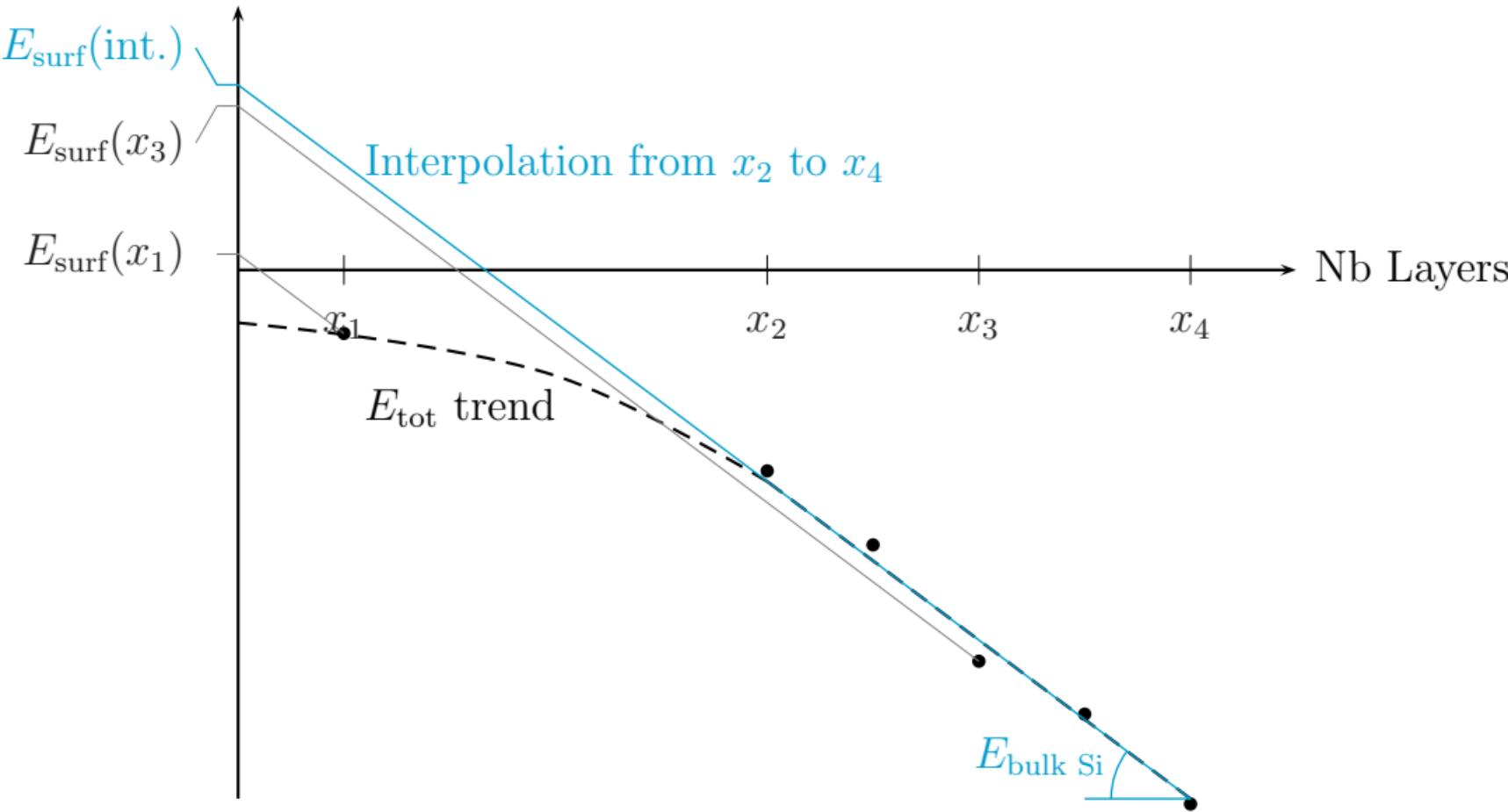
Surface Energy [meV/ \AA^2]



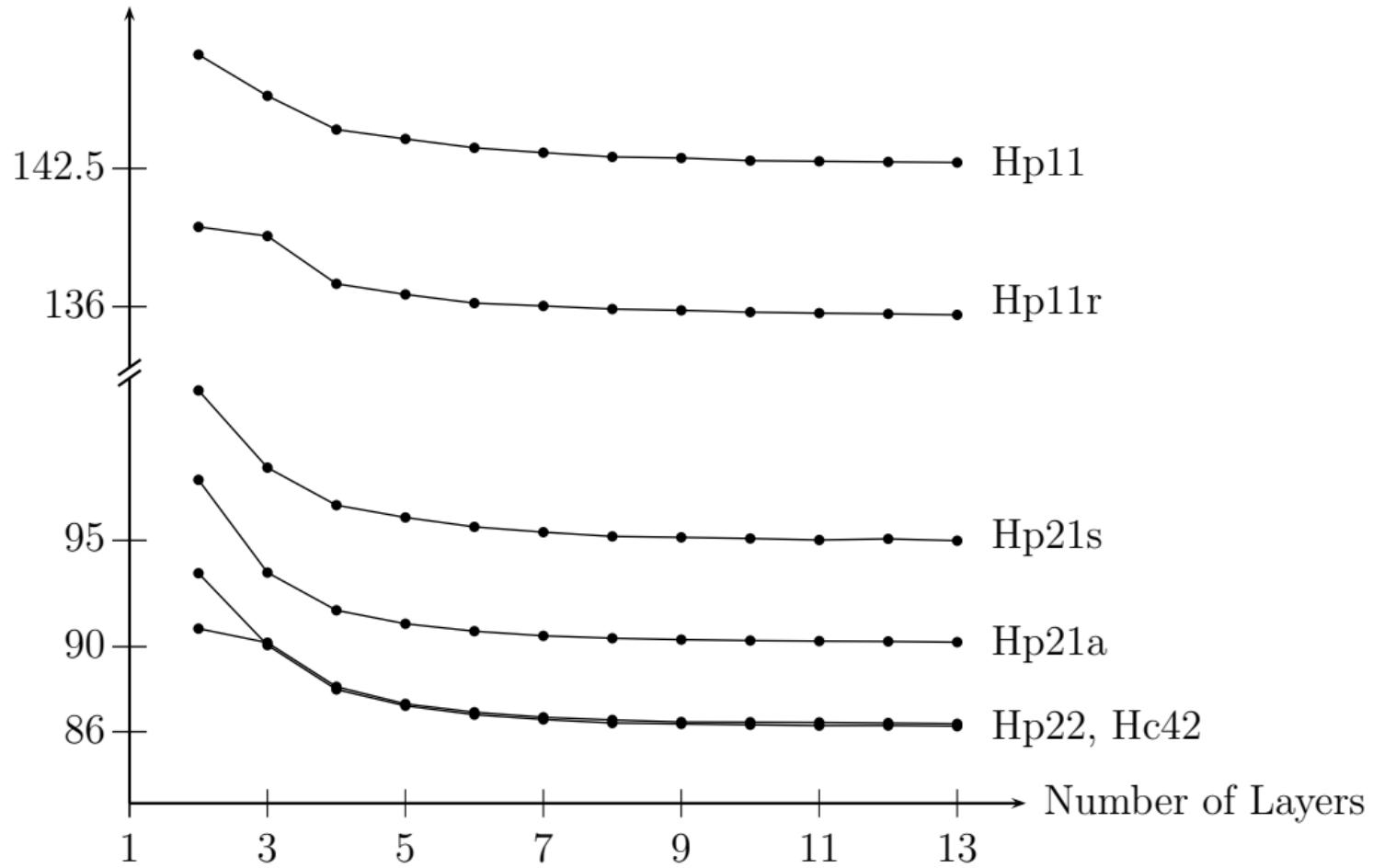
Surface Energy [meV/ \AA^2]

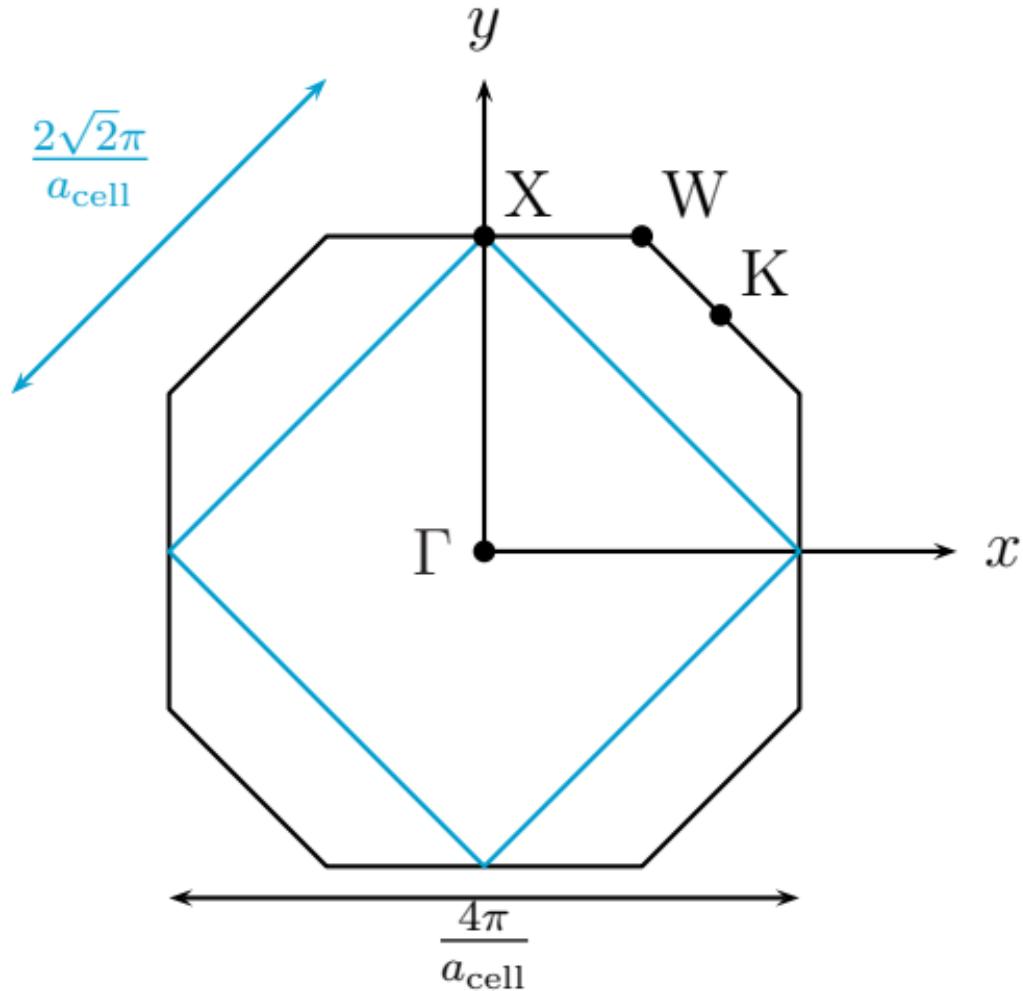


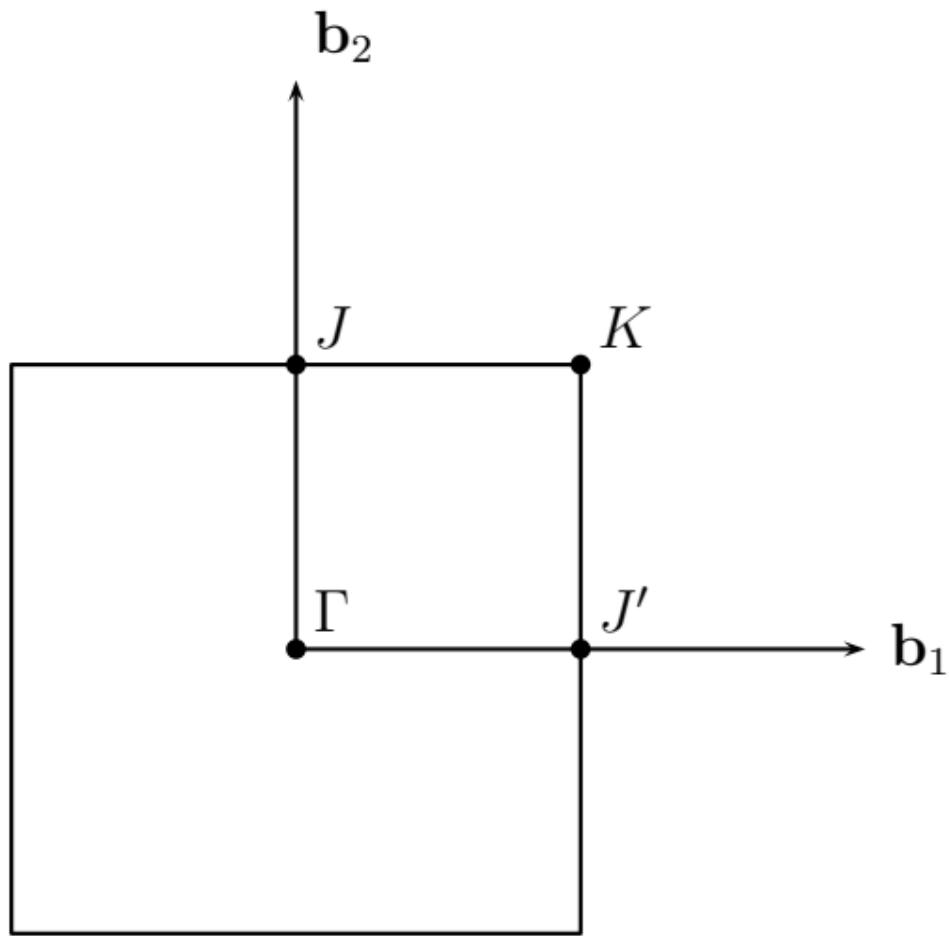
Total Energy



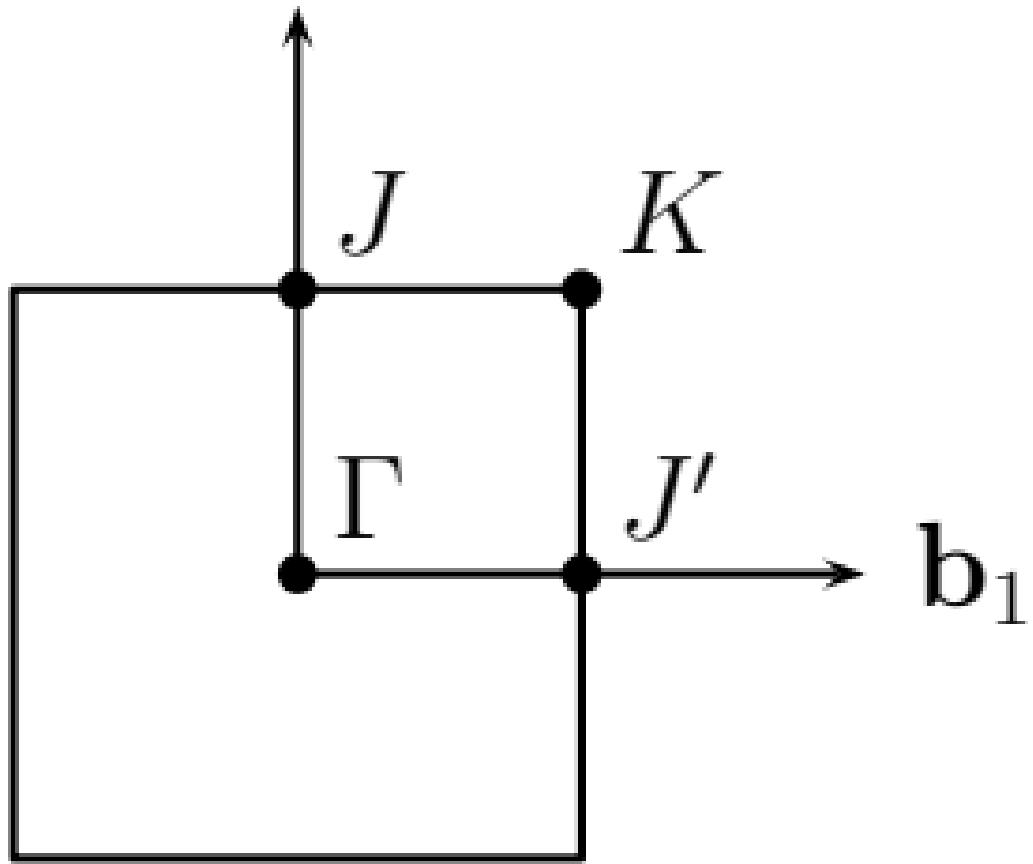
Surface Energy [meV/ \AA^2]

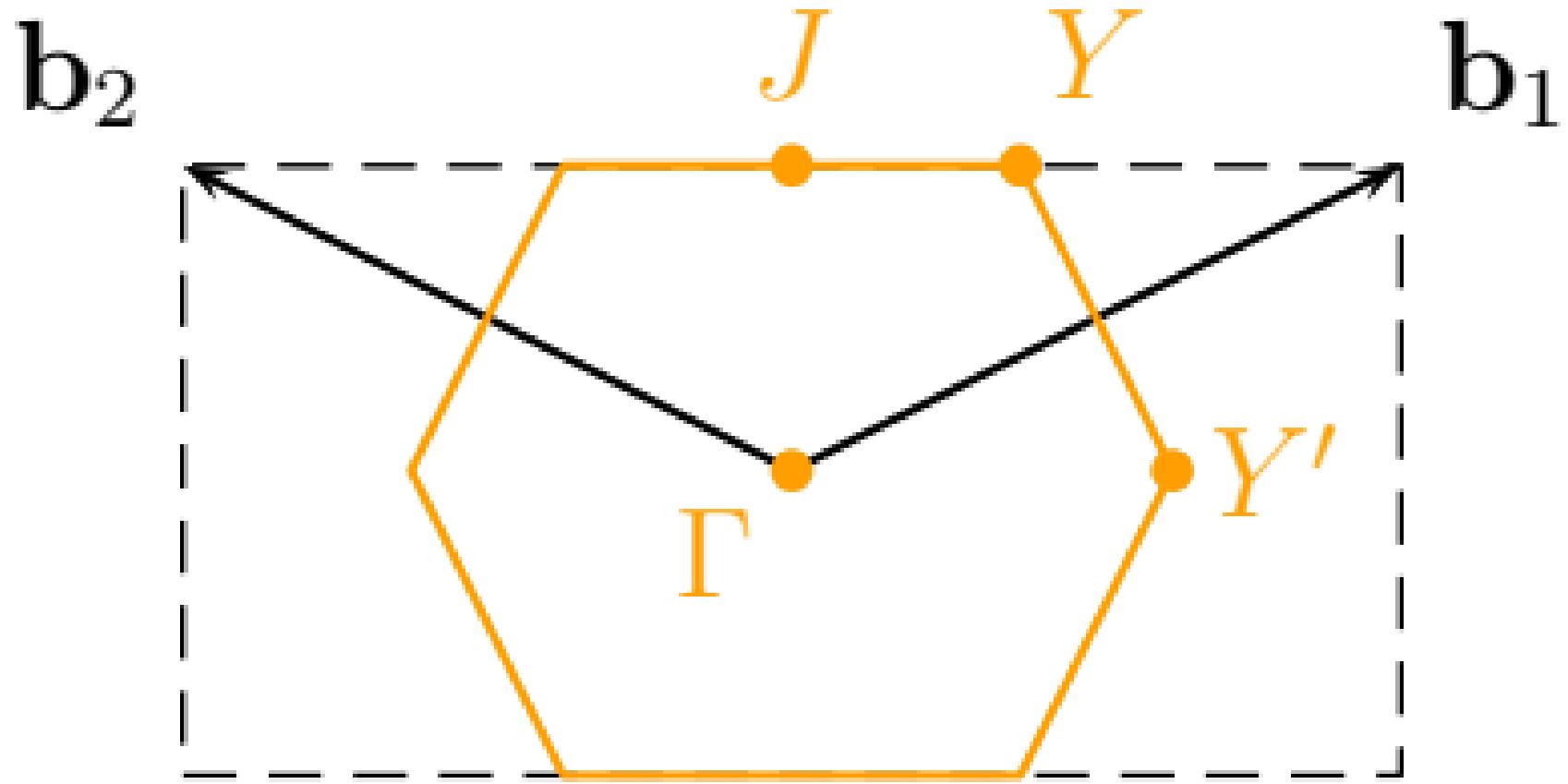


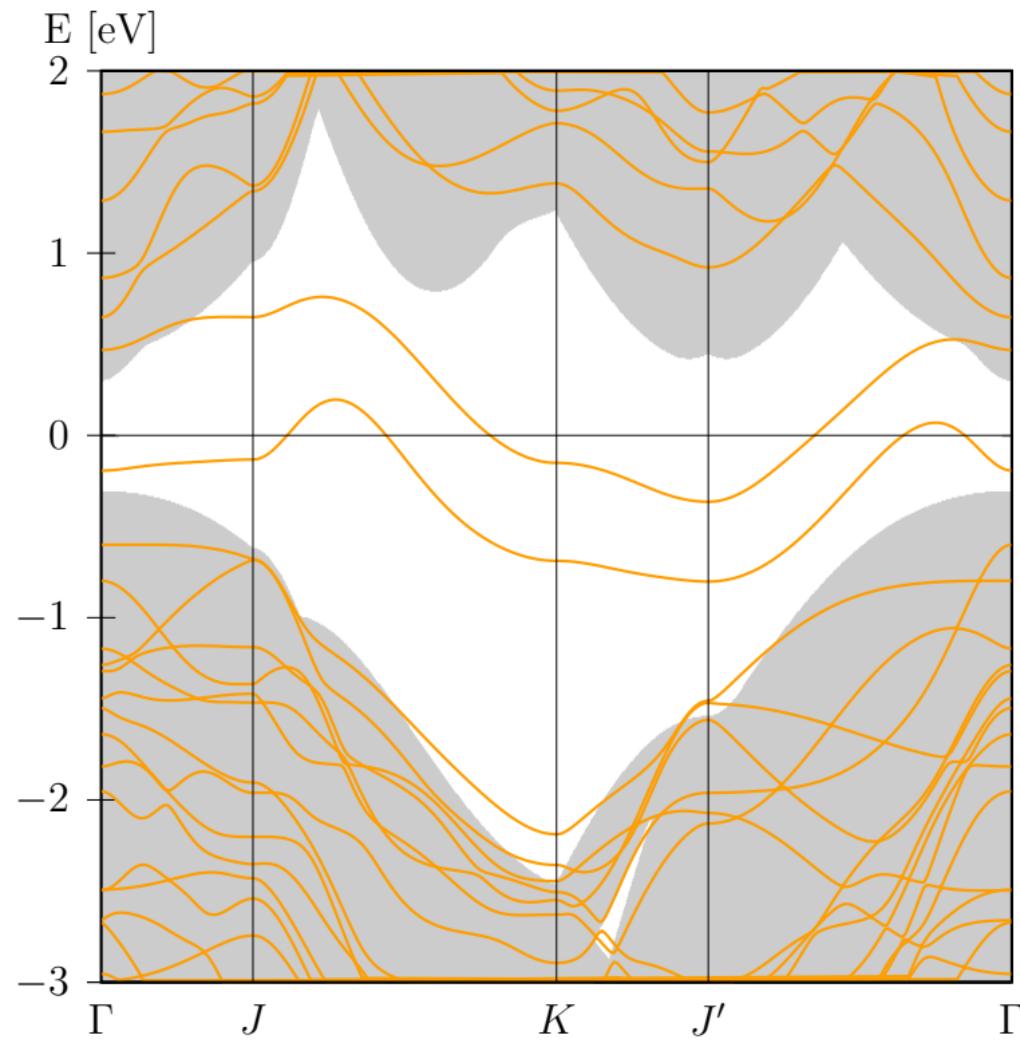




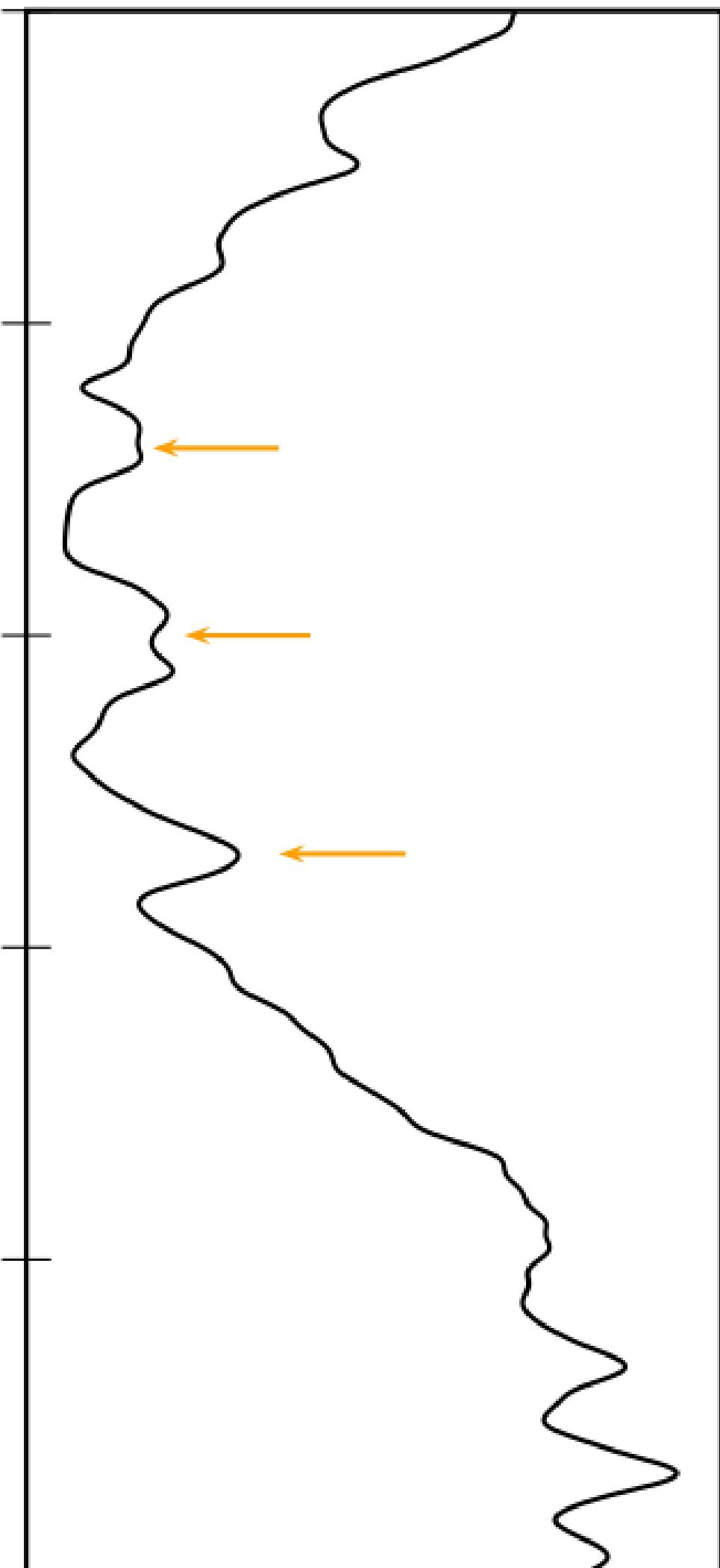
b_2  J K  Γ J'  b_1

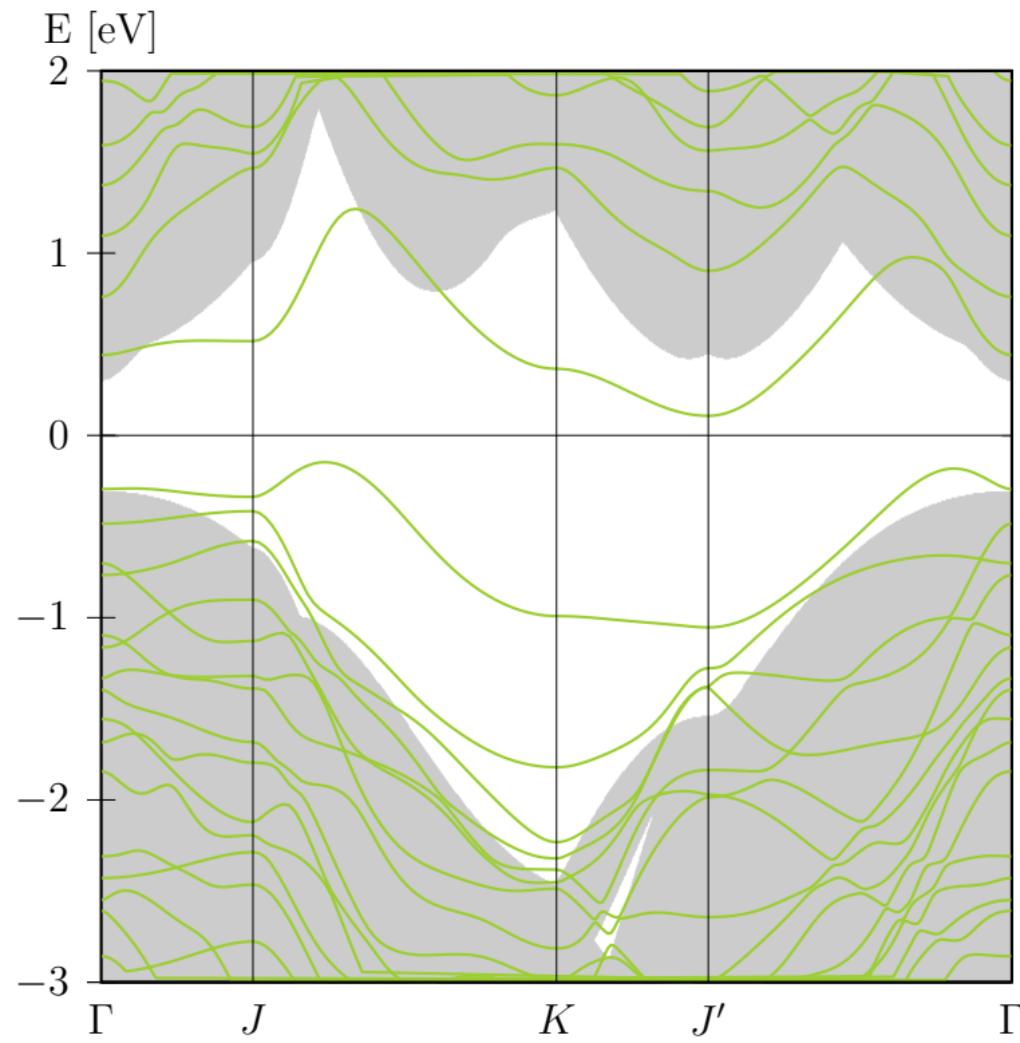
b_2 



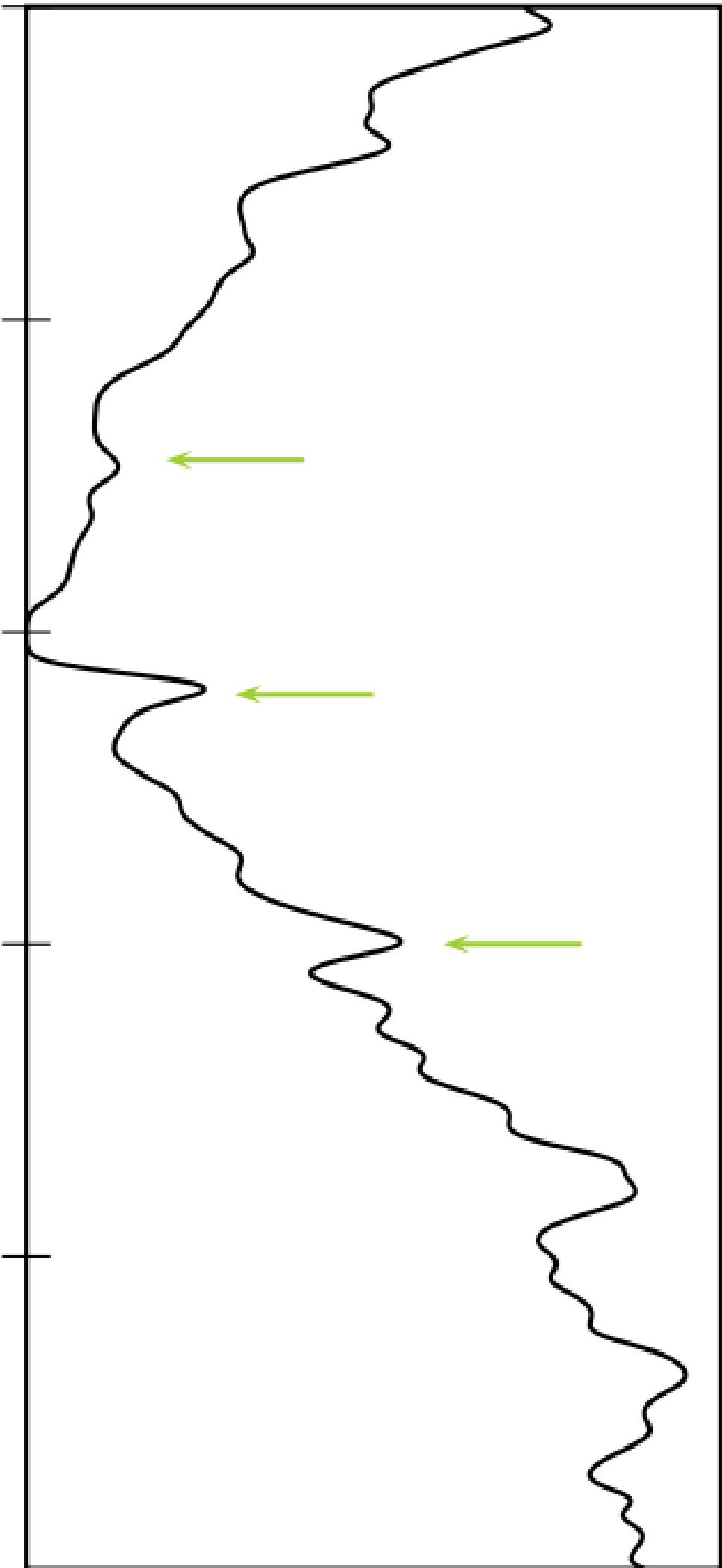


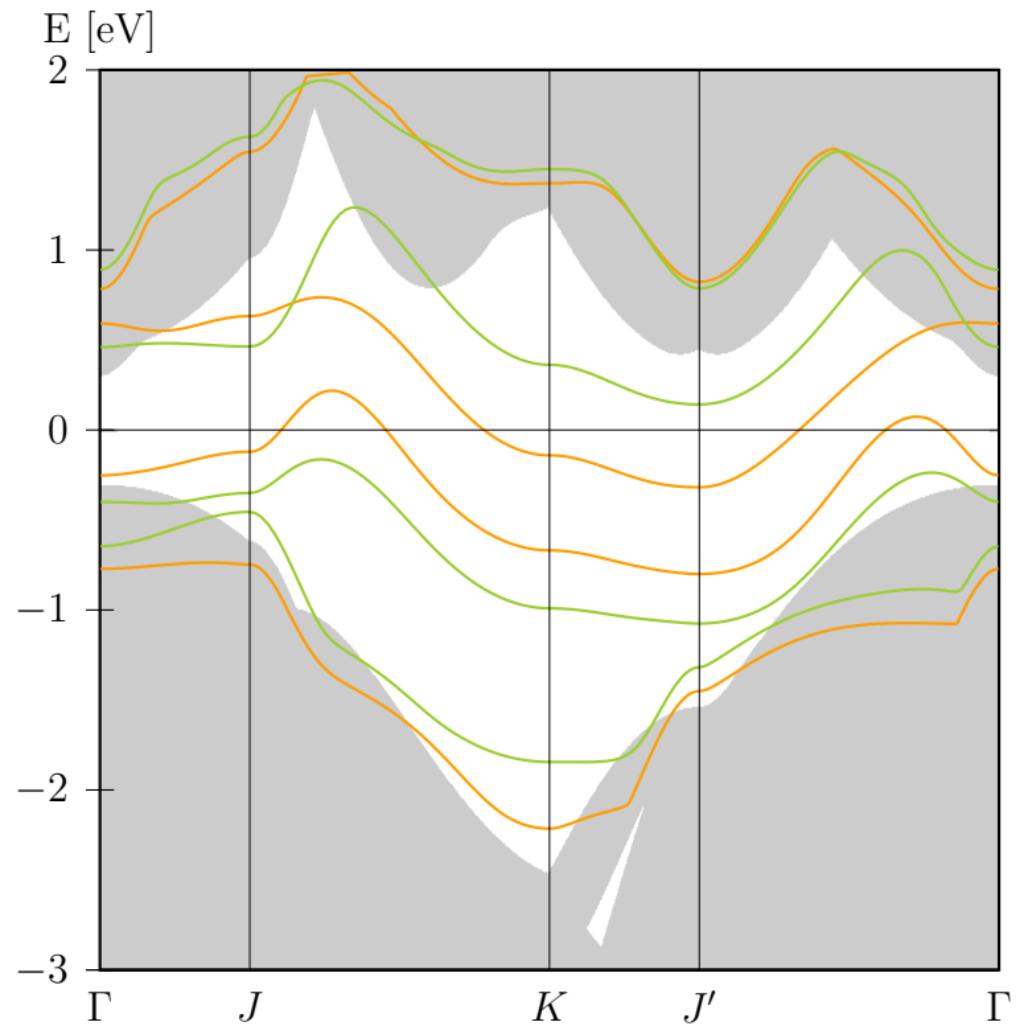
DOS [a.u.]





DOS [a.u.]





E [eV]

2

1

0

-1

-2

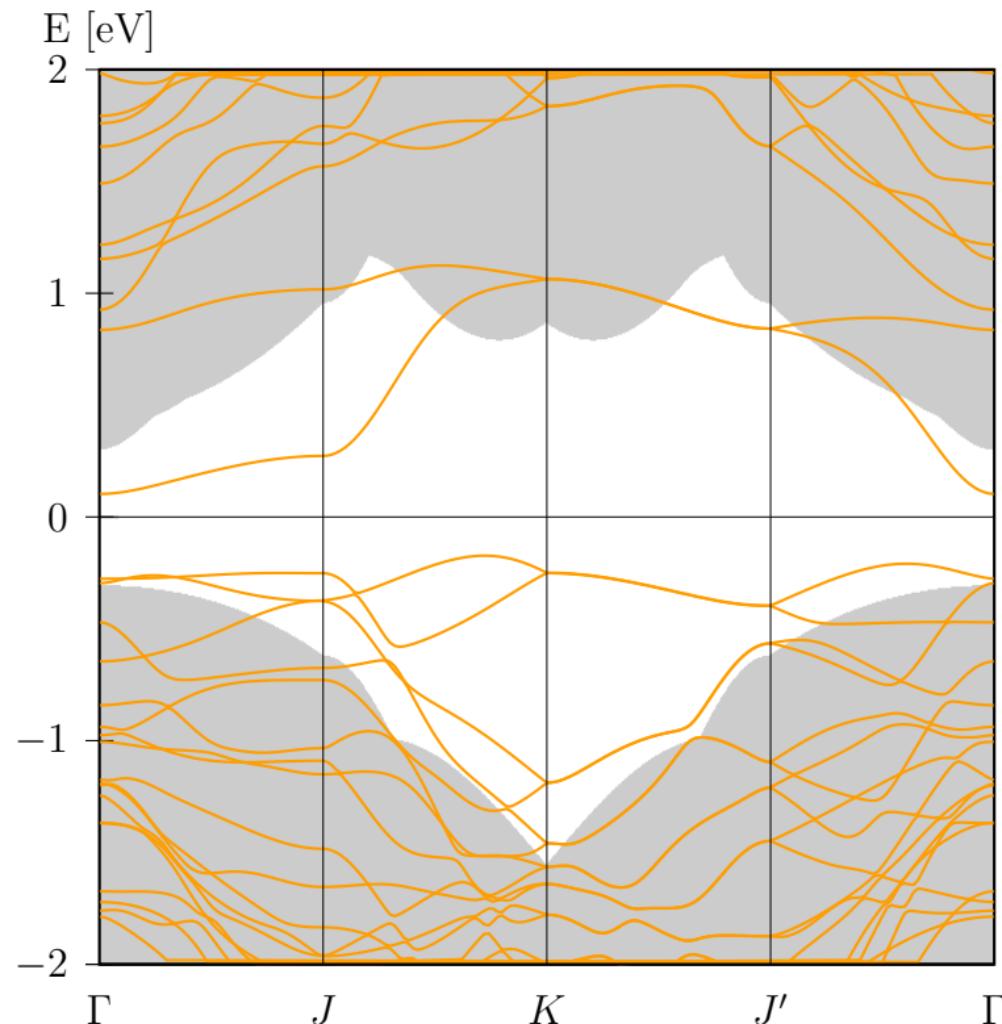
Γ

J

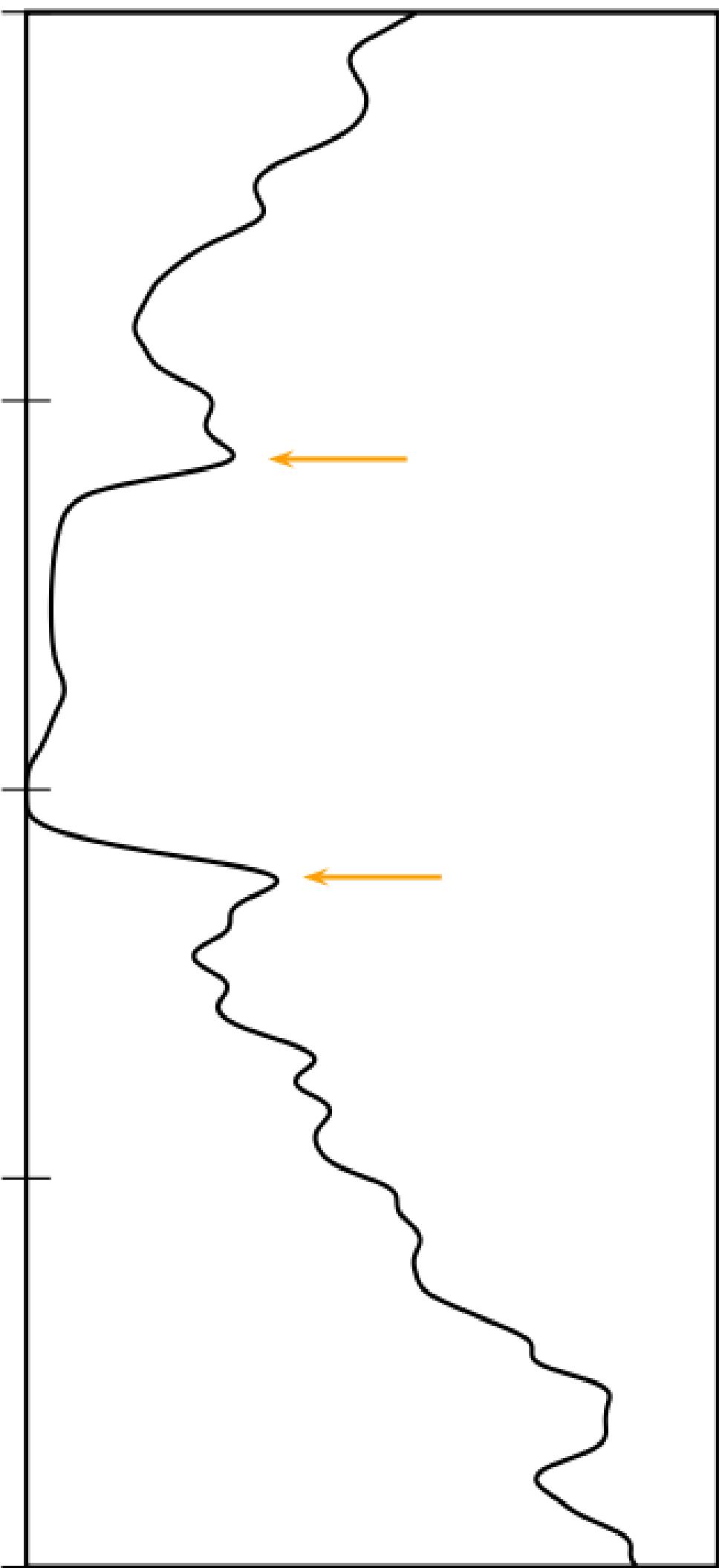
K

J'

Γ



DOS [a.u.]



E [eV]

2

1

0

-1

-2

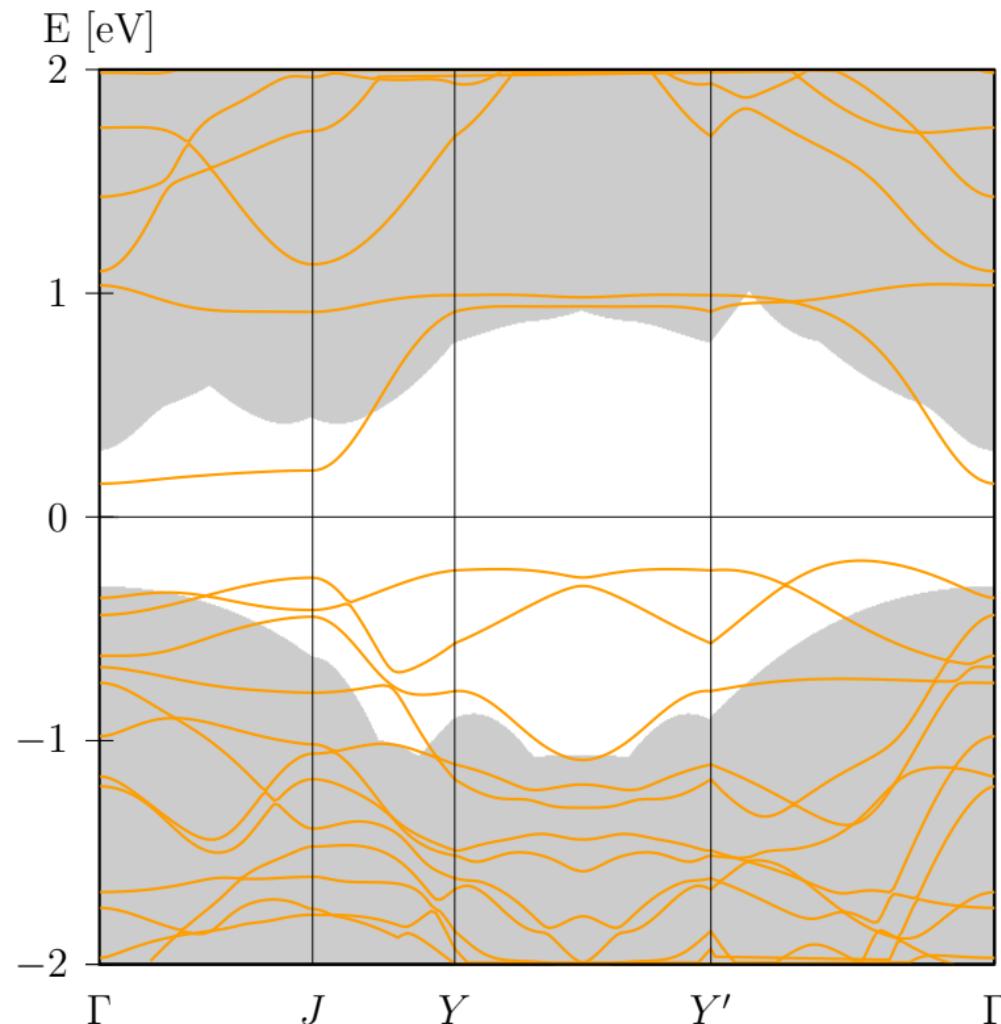
Γ

J

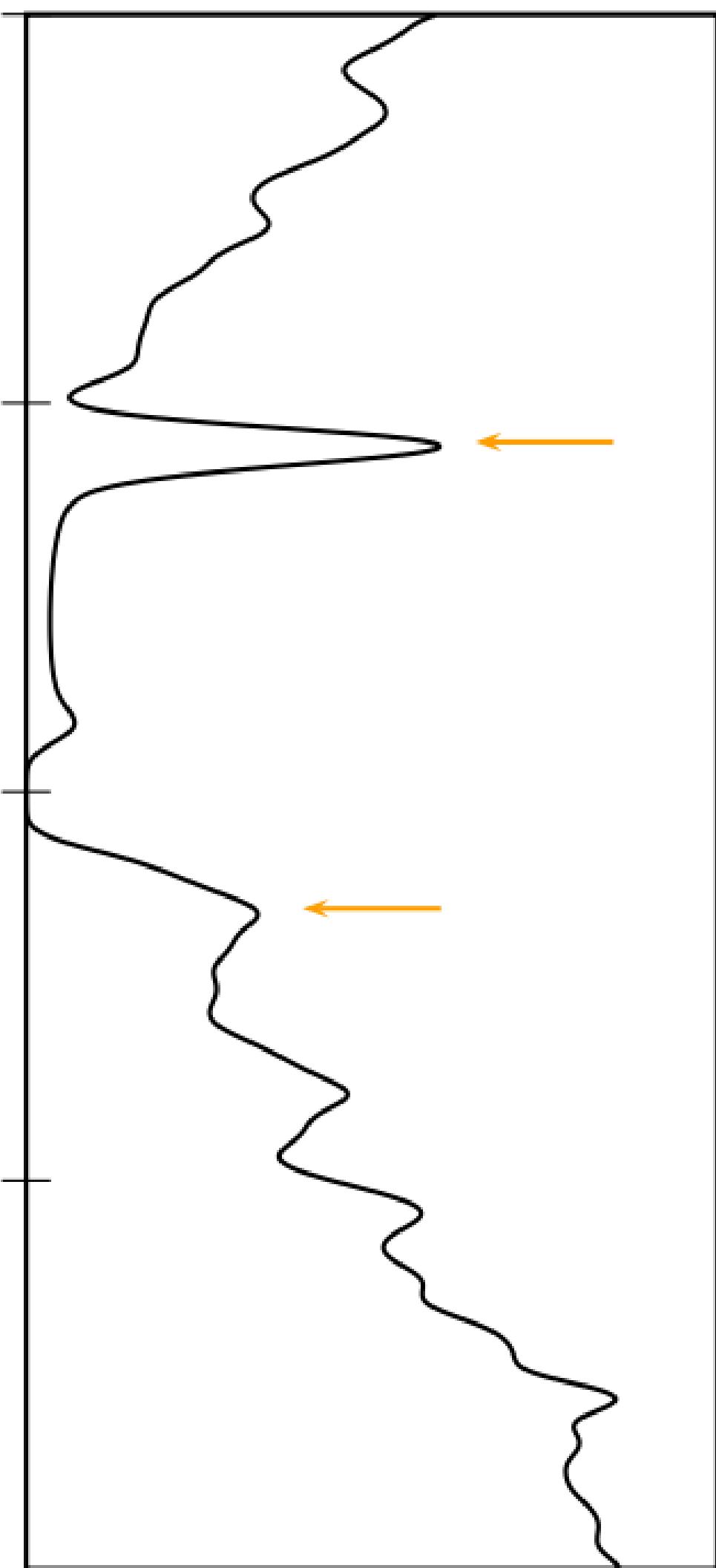
Y

Y'

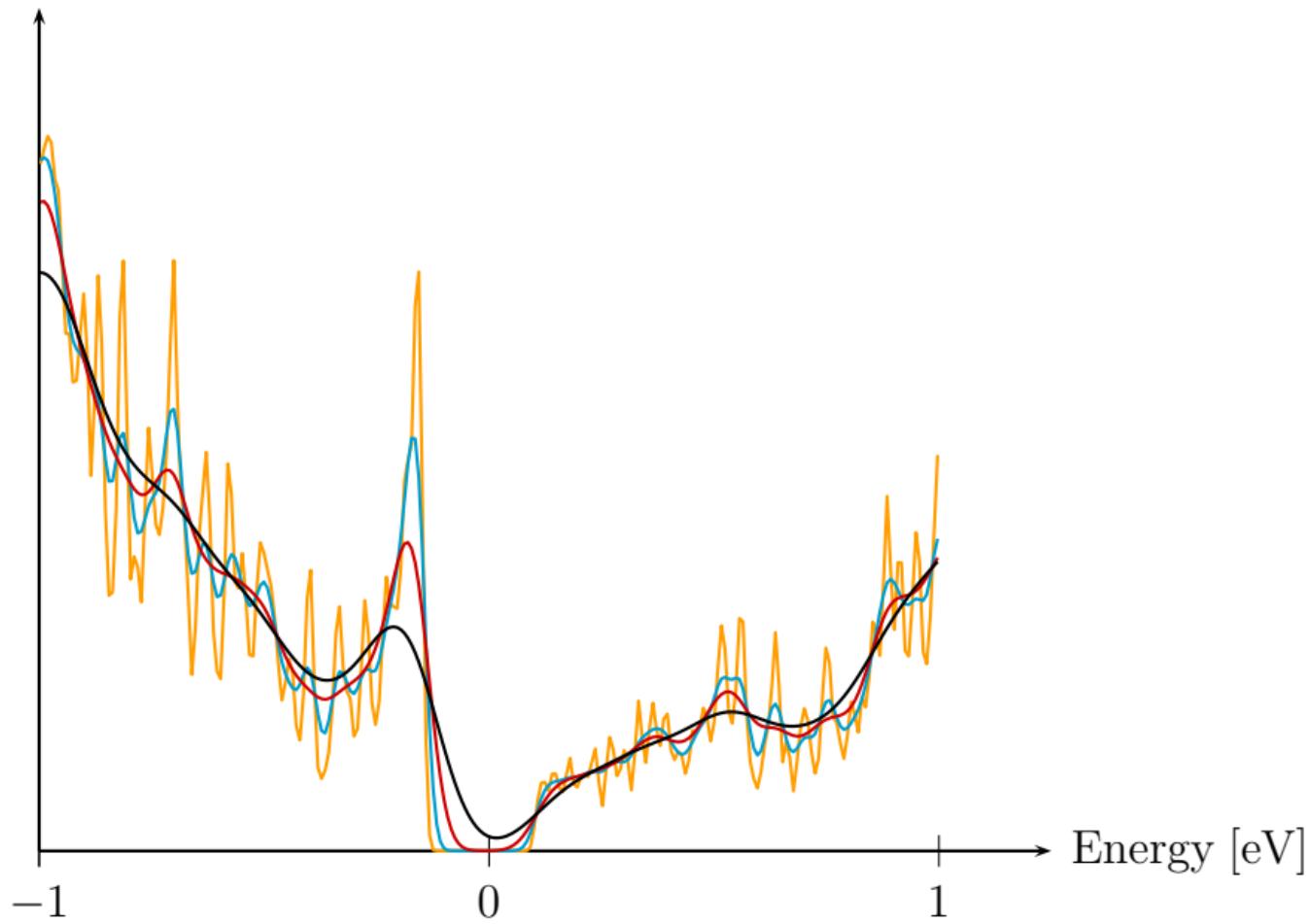
Γ



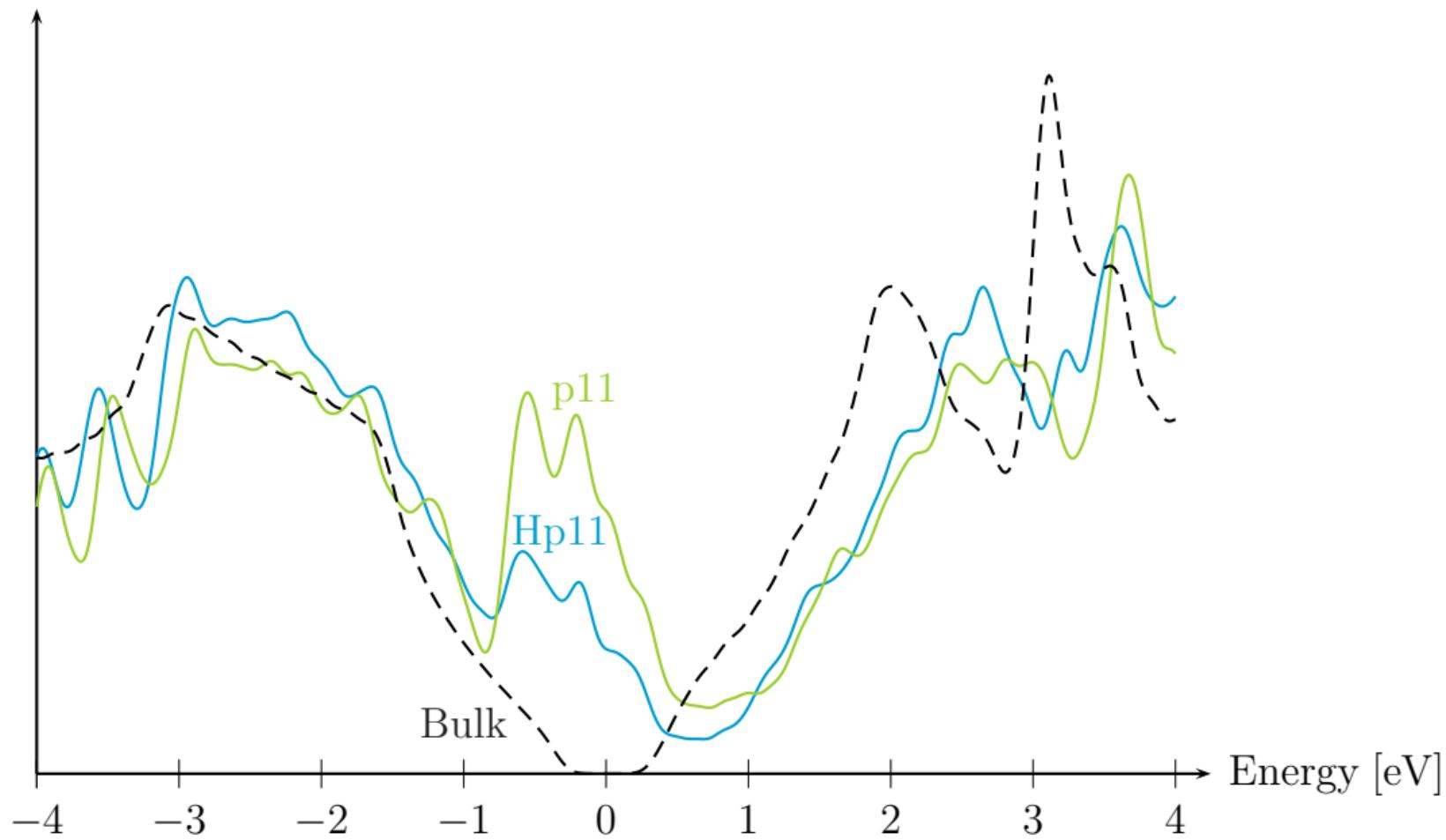
DOS [a.u.]



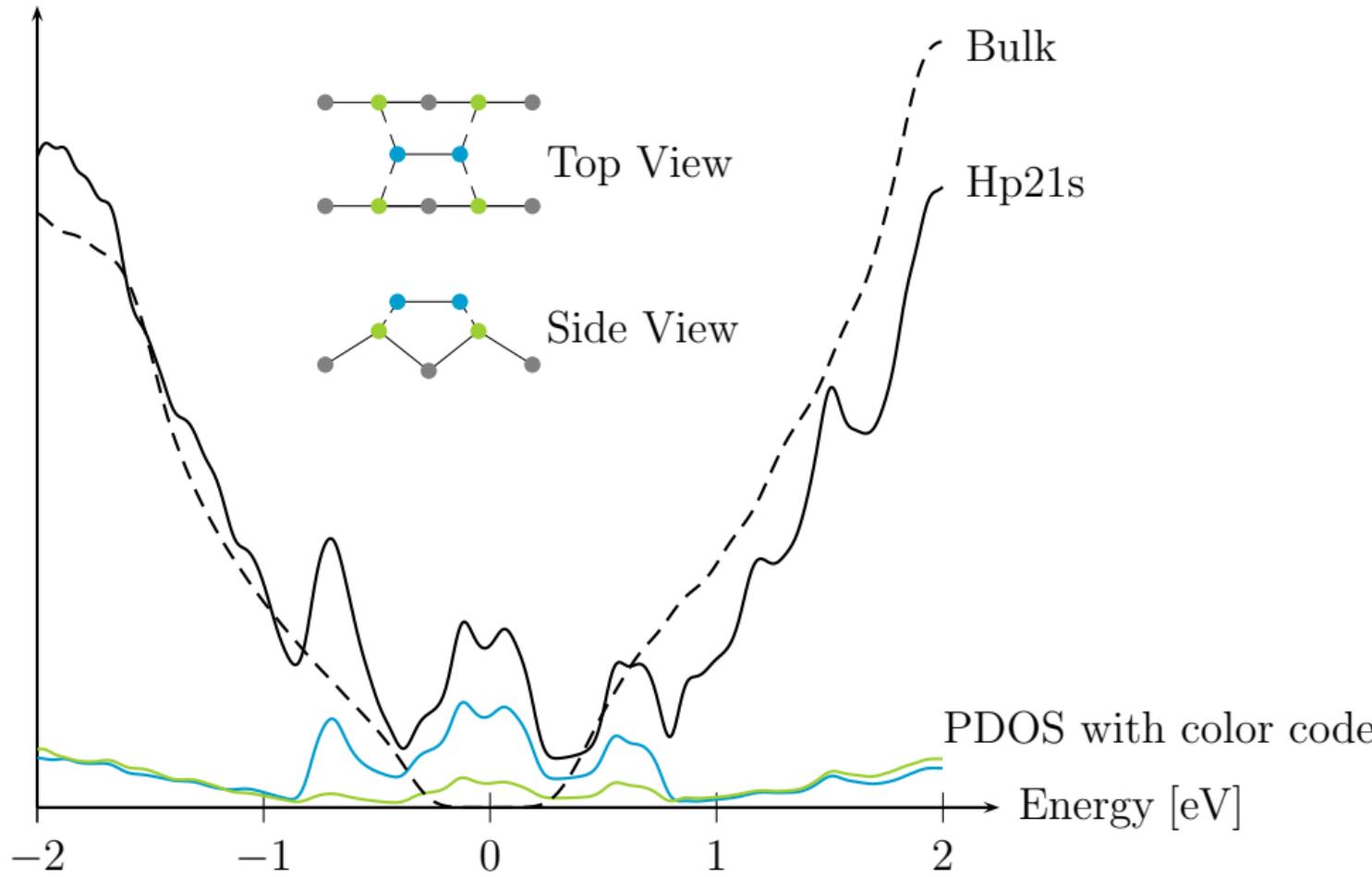
DOS [a.u.]



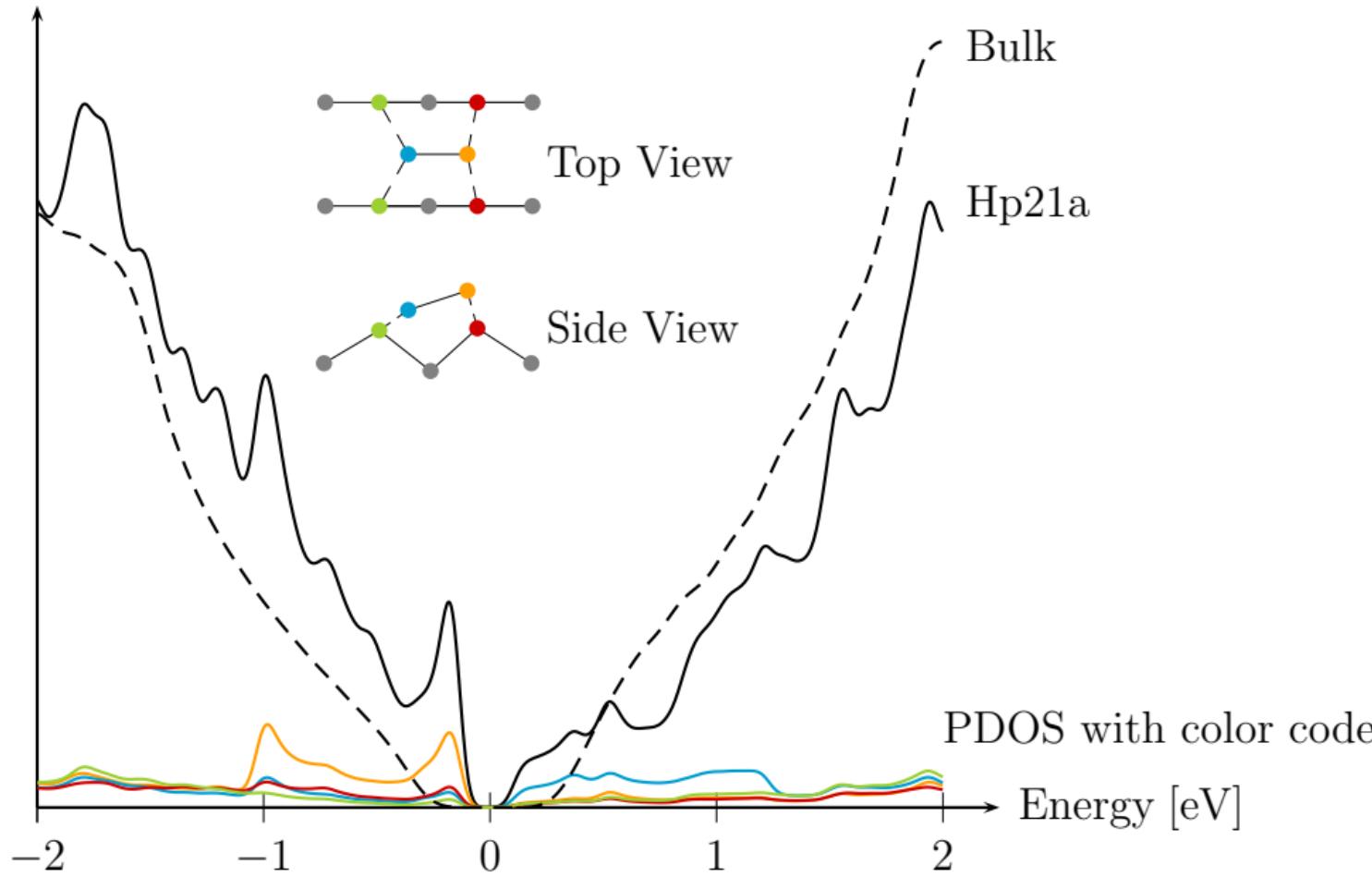
DOS [a.u.]



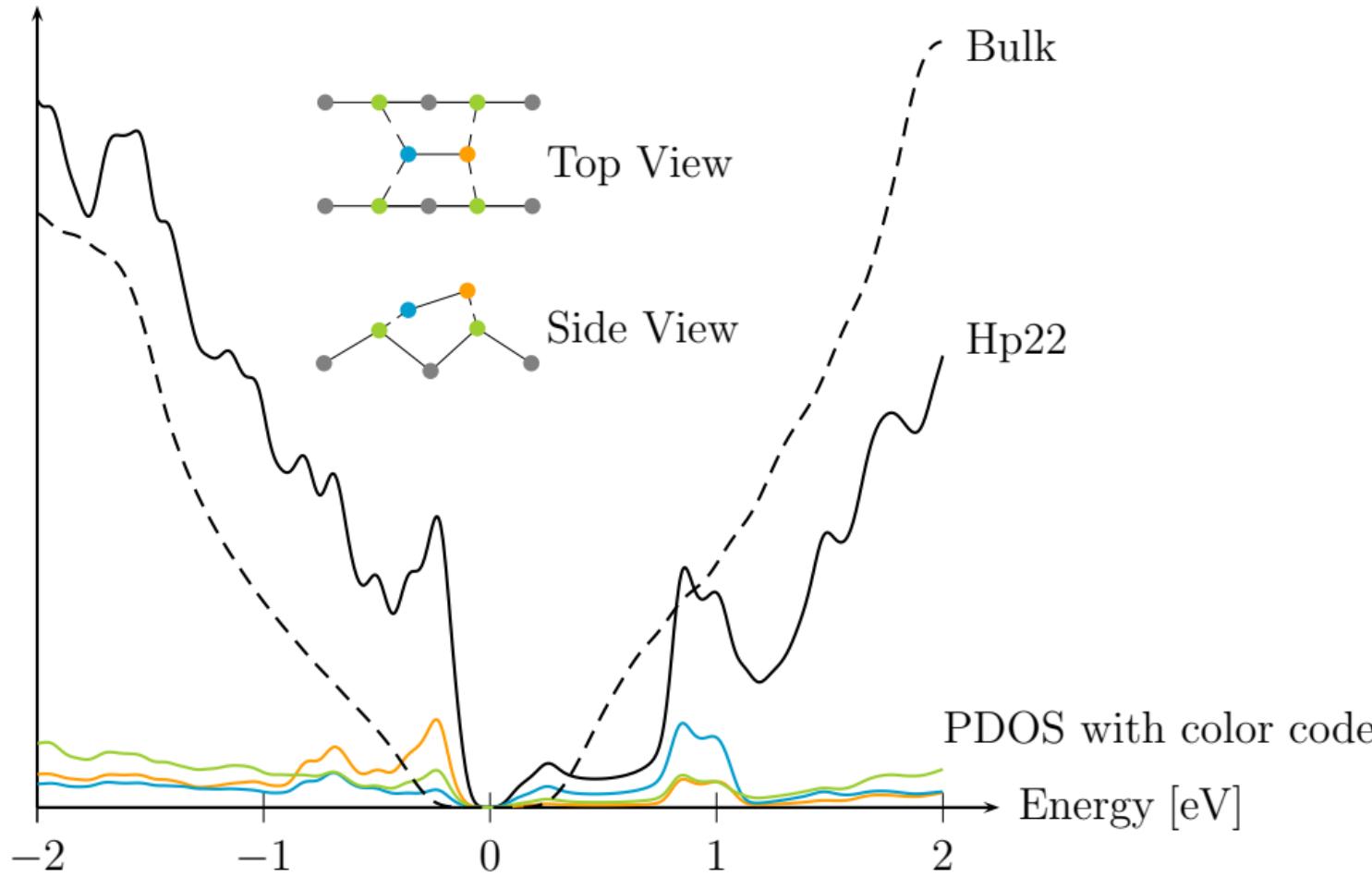
(P)DOS [a.u.]



(P)DOS [a.u.]



(P)DOS [a.u.]



(P)DOS [a.u.]

