Курс: Електронна структура та властивості низькорозмірних систем

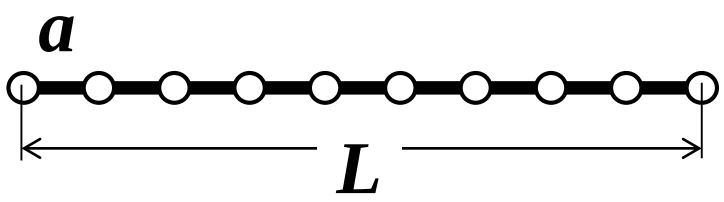
Лектор: Олександр Кордюк

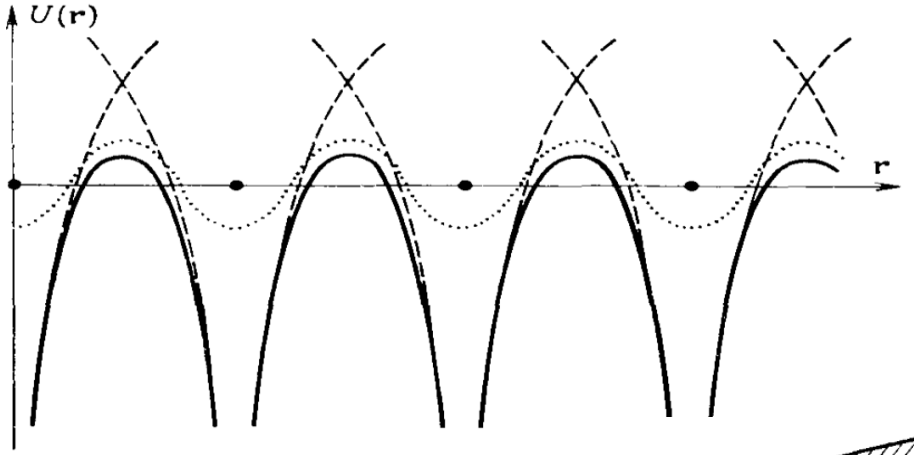
Лекція 4: **Перехід Паєрлса**

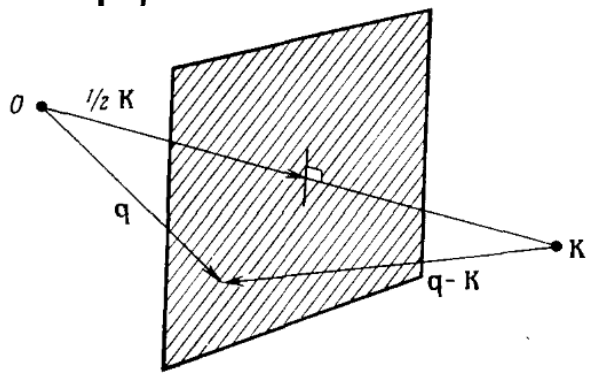
- Висновки попередньої лекції: зонна щілина, ширина зони, метал чи ізолятор.
- Ще про представлення 2- та 3-вимірної дисперсії.
- Ефект димеризації - нова зонна щілина.
- 7x7 надструктура поверхні кремнію.
- Нестинг поверхонь Фермі: 1D, 2D, 3D.

Band gaps

У попередніх лекціях…



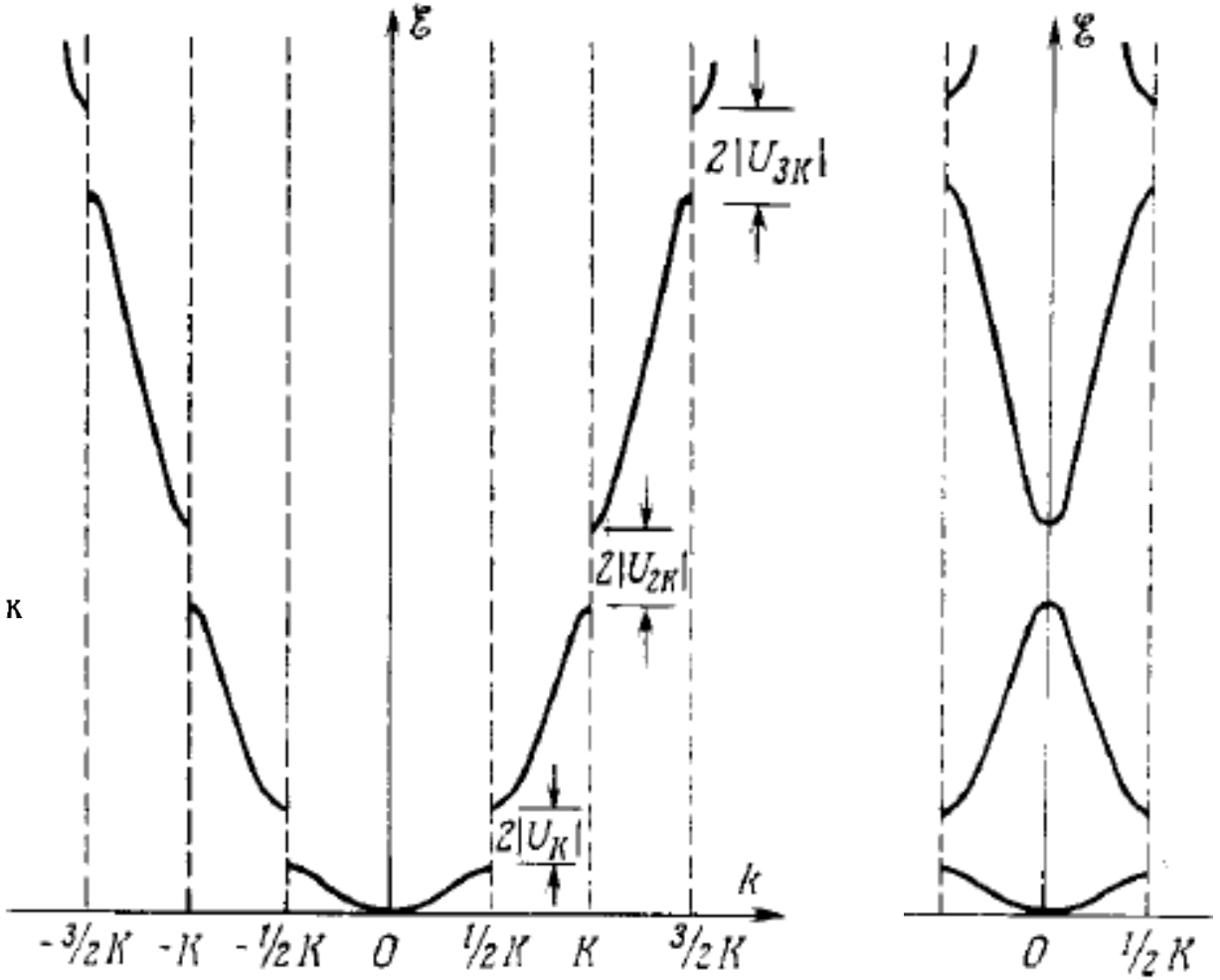




$$\begin{vmatrix} \mathscr{E} - \mathscr{E}^0_{\mathbf{q}} & -U_{\mathbf{K}} \\ -U^*_{\mathbf{K}} & \mathscr{E} - \mathscr{E}^0_{\mathbf{q}-\mathbf{K}} \end{vmatrix} = 0$$

$$(\mathscr{E} - \mathscr{E}^0_{\mathbf{q}})\,(\mathscr{E} - \mathscr{E}^0_{\mathbf{q}-\mathbf{K}}) = |U_{\mathbf{K}}|^2$$

$$\mathscr{E} = \frac{1}{2}\,(\mathscr{E}^0_{\mathbf{q}} + \mathscr{E}^0_{\mathbf{q}-\mathbf{K}}) \pm \left[\left(\frac{\mathscr{E}^0_{\mathbf{q}} - \mathscr{E}^0_{\mathbf{q}-\mathbf{K}}}{2}\right)^2 + |U_{\mathbf{K}}|^2\right]^{1/2}$$

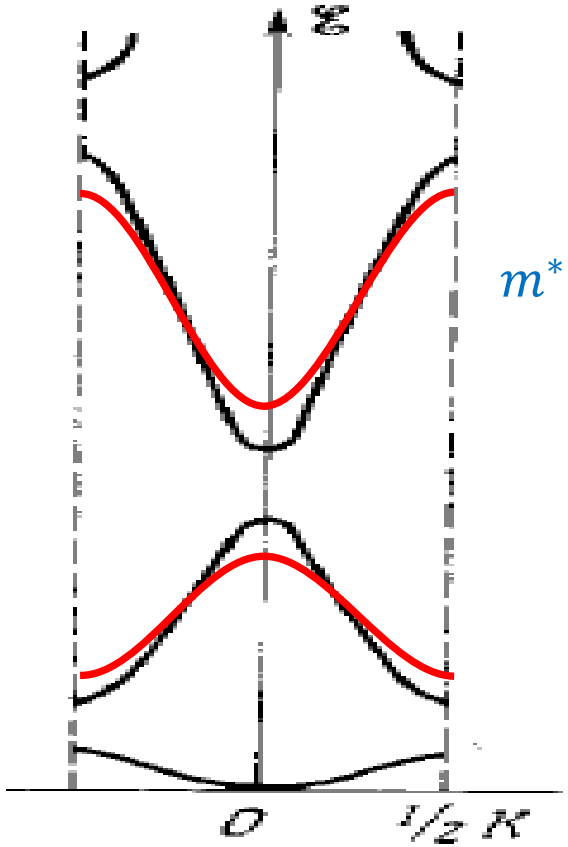


$K = 2\pi/a$

Наближення слабкого зв’язку

$$\mathscr{E} = \frac{1}{2}\left(\mathscr{E}^0_{\mathbf{q}} + \mathscr{E}^0_{\mathbf{q}-\mathbf{K}}\right) \pm \left[\left(\frac{\mathscr{E}^0_{\mathbf{q}} - \mathscr{E}^0_{\mathbf{q}-\mathbf{K}}}{2}\right)^2 + |U_{\mathbf{K}}|^2\right]^{1/2}$$

>U

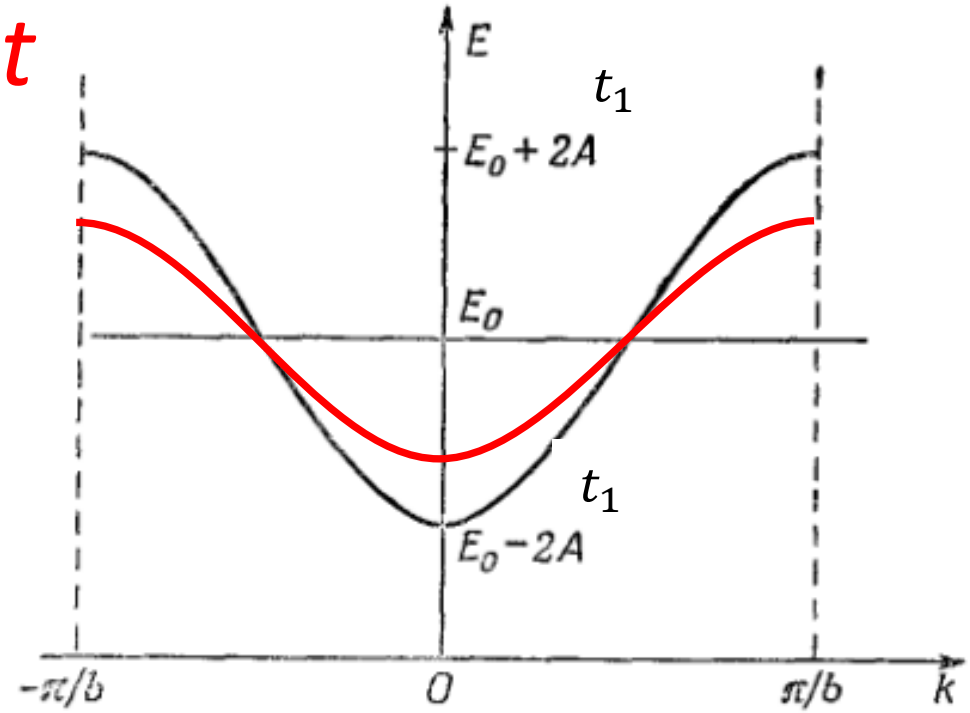


$$m^* = \pm\frac{a^2 m^2 |U_{nK}|}{(n\pi)^2}$$

Модель перескоків

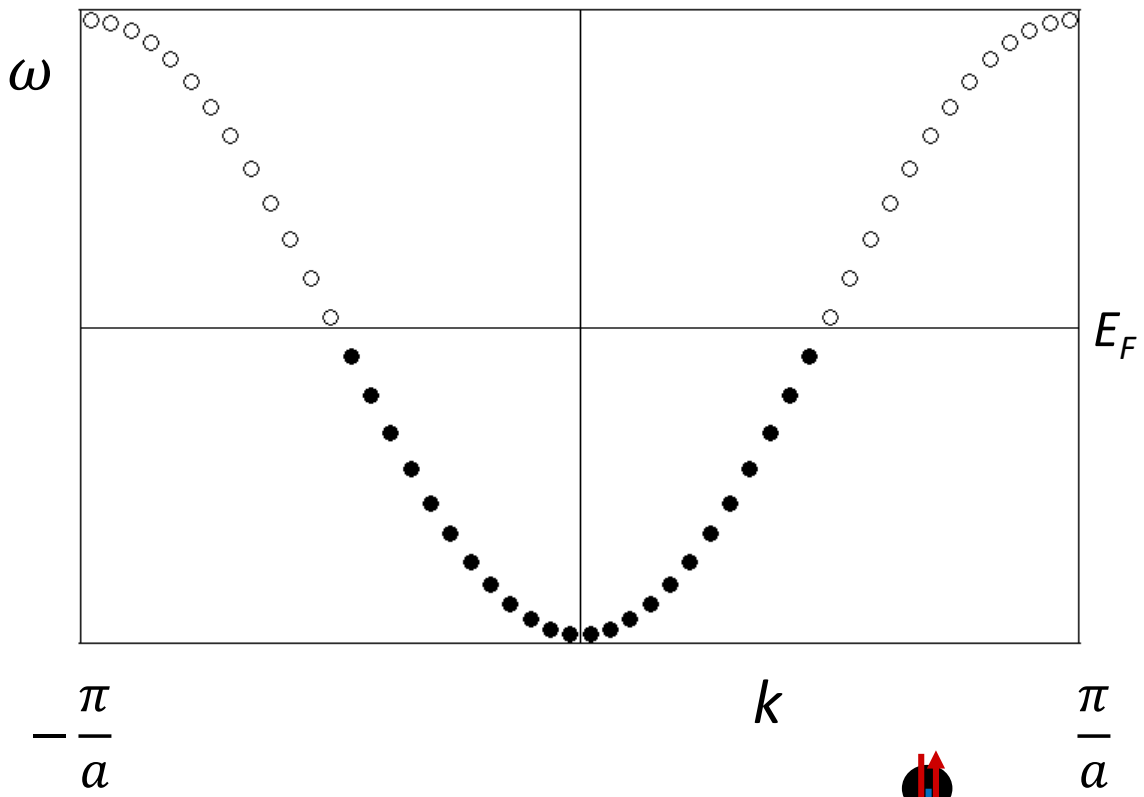
$$E = E_0 + t_1 \cos(ak) + t_2 \cos(2ak) + \ldots$$

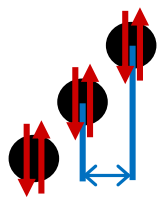
< t



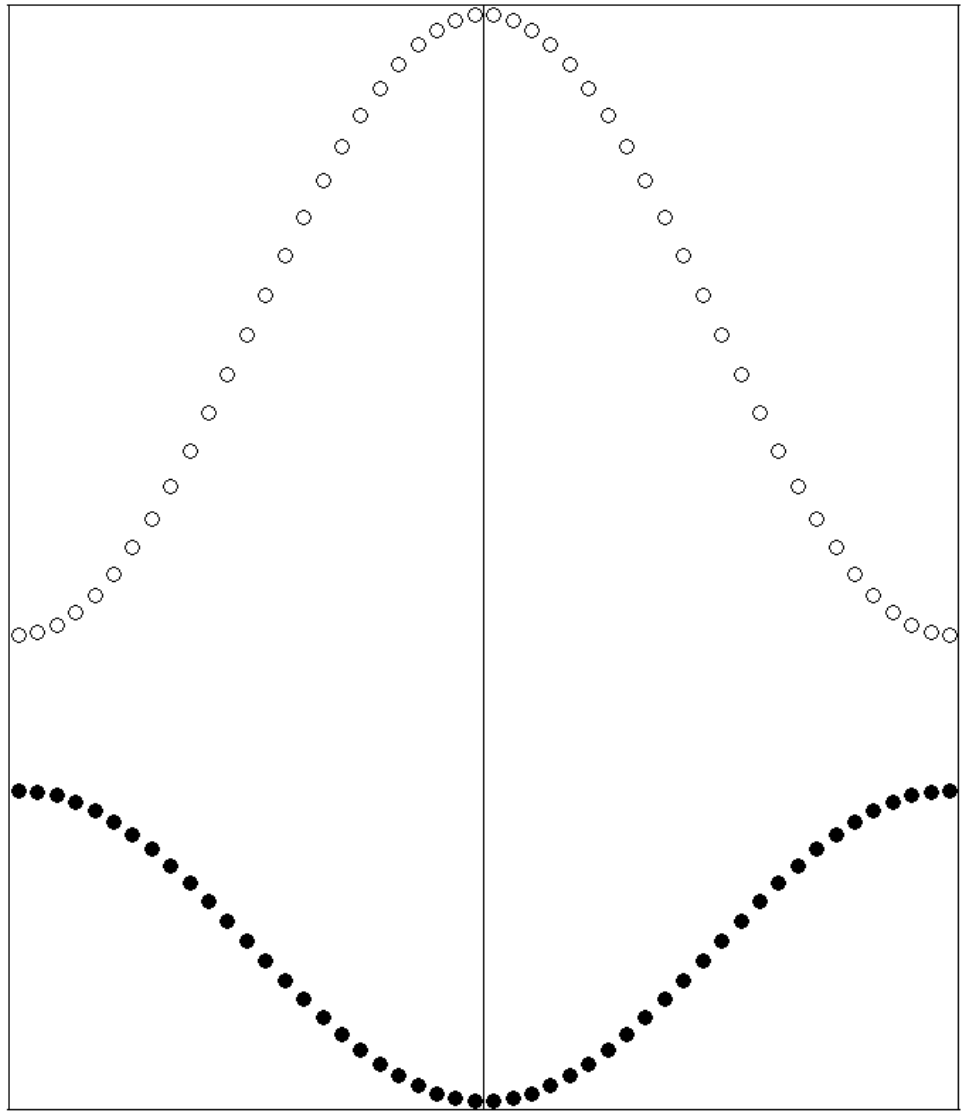
$$m^* = -a^2 t$$

Metal *vs* Insulator



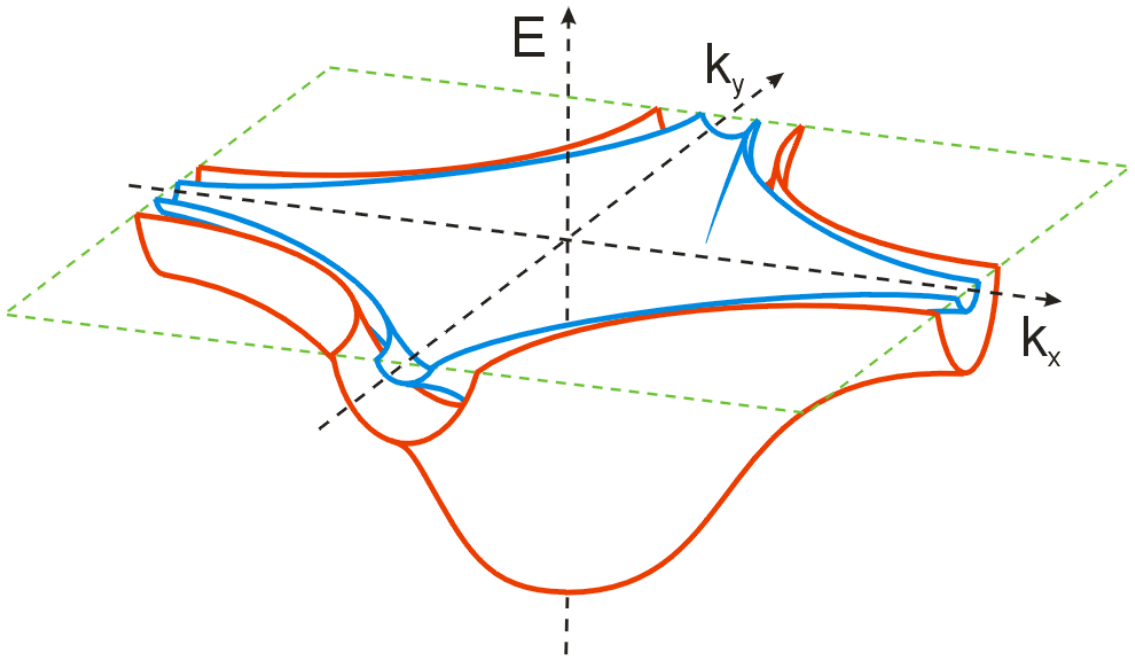


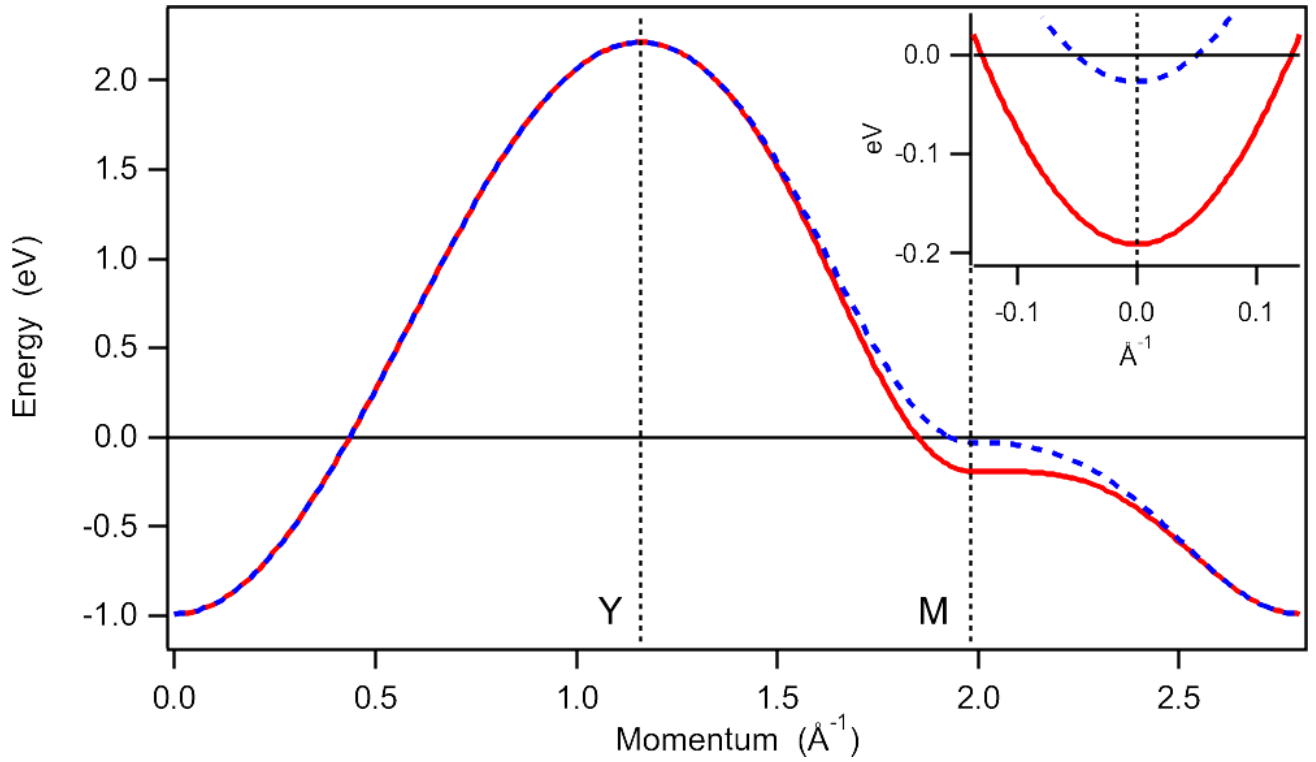
$dk = 2\pi/L$



Модель перескоків в 2D

$$E = E_0 + t_1\left(\cos(ak_x) + \cos(ak_y)\right) + t_2\left(\cos(2ak_x) + \cos(2ak_y)\right) + \ldots$$





Kordyuk *PRB* 2003

Developed with support from NSF-IUSE #1524968.

E

F

Graph | 3D Mode

x = 1.963

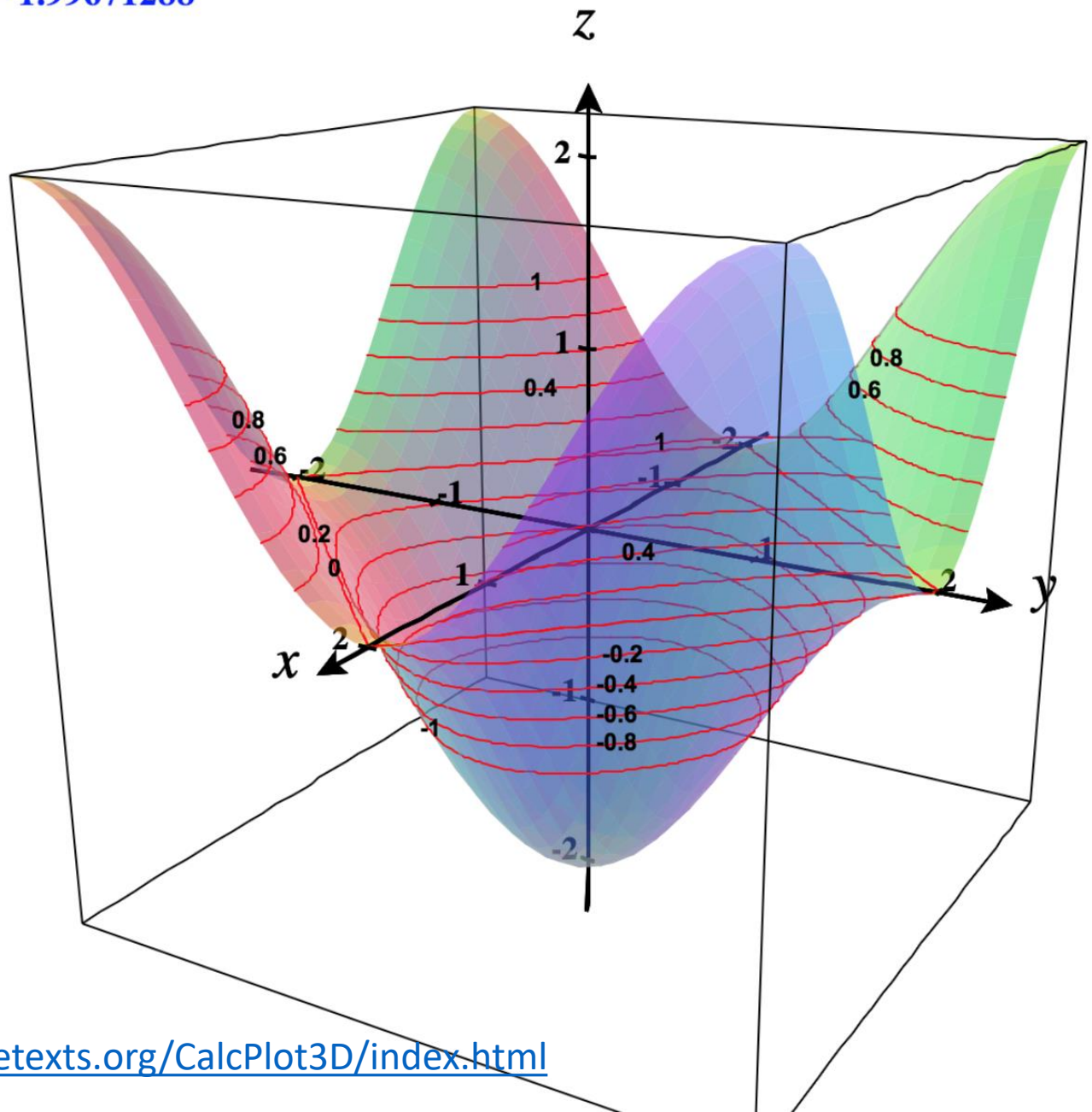
y = 1.963

Add to graph: Select...

z = -cos(pi*x/2)-cos(pi*y/2)

Number of Gridlines 30

$f(1.9635, 1.9635) = 1.99671288$



https://c3d.libretexts.org/CalcPlot3D/index.html

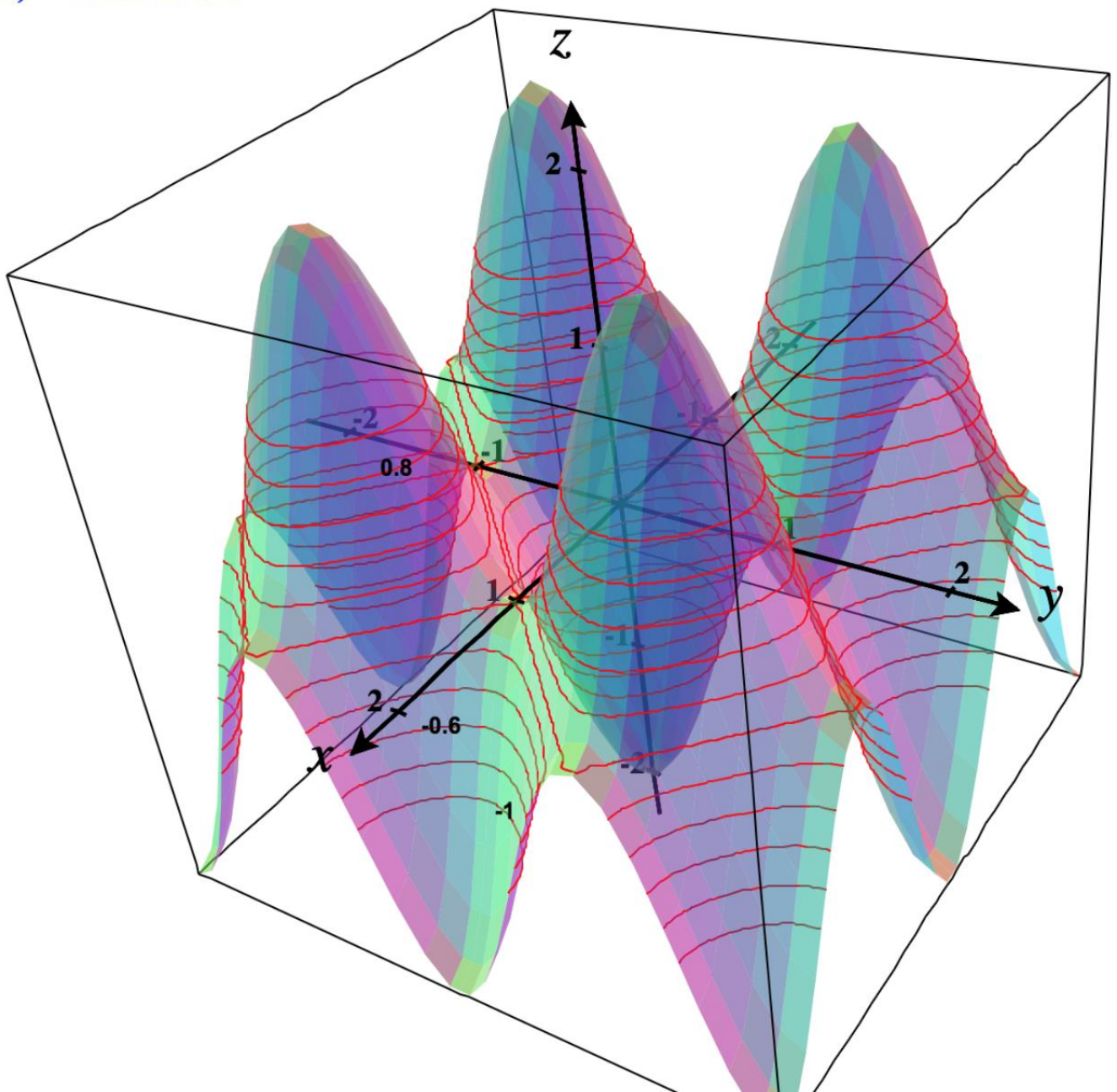
Developed with support from NSF-IUSE #1524968.

E

F

Graph | 3D Mode

$f(1.9635, 1.9635) = 1.99671288$



$x =$ 1.963

$y =$ 1.963

Add to graph: Select...

$z =$ -cos(2*pi*x/2)-cos(2*pi*y/2)

Number of Gridlines 30

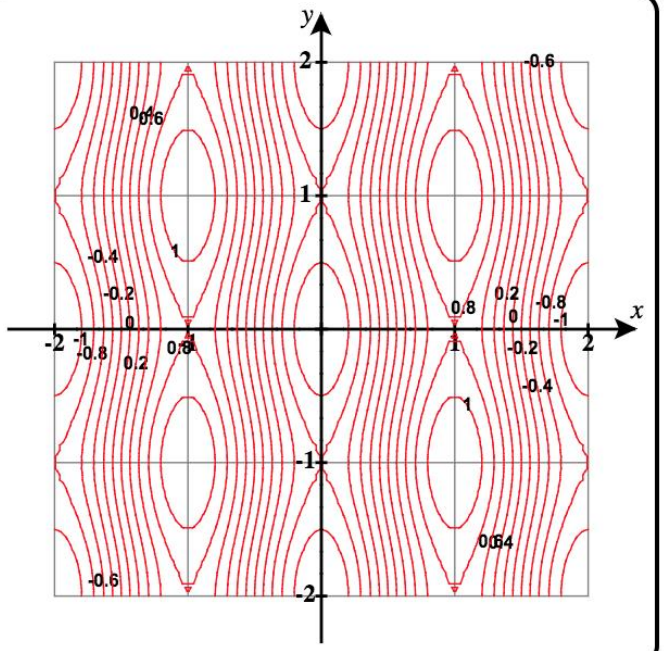
Developed with support from NSF-IUSE #1524968.

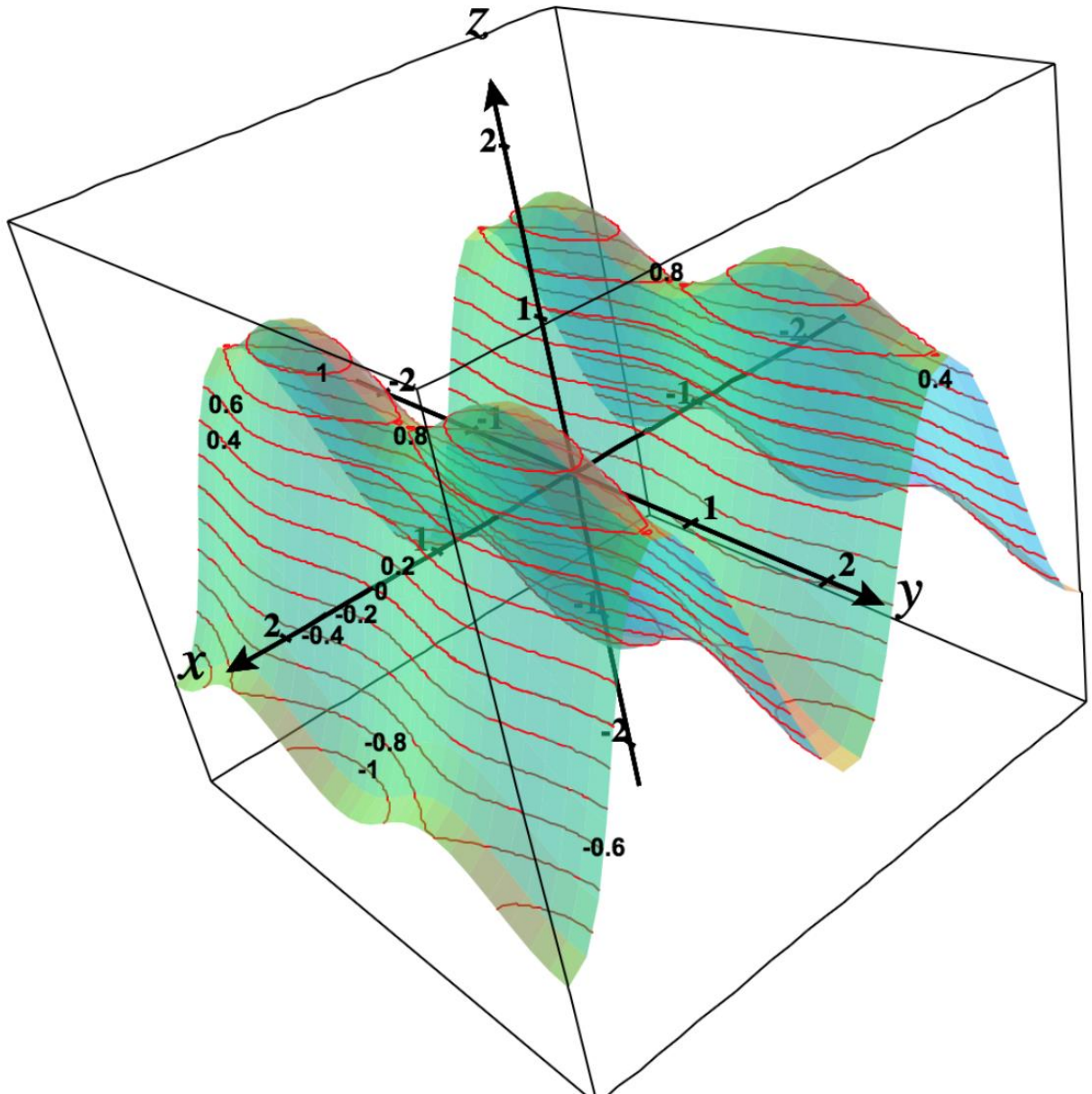
E

F

Graph | 3D Mode

$f(1.9635, 1.9635) = 1.99671288$





x = 1.963

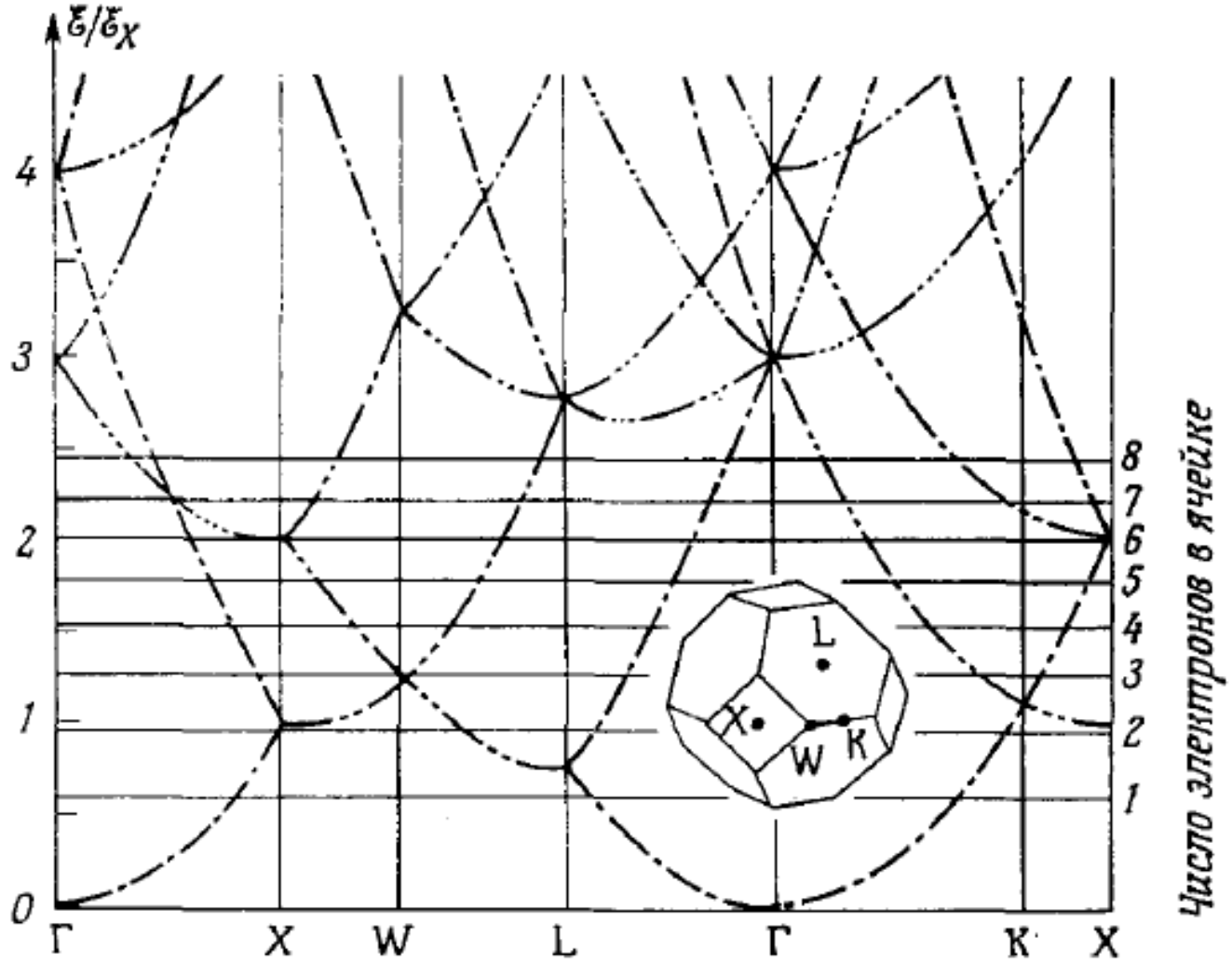
y = 1.963

Add to graph: Select...

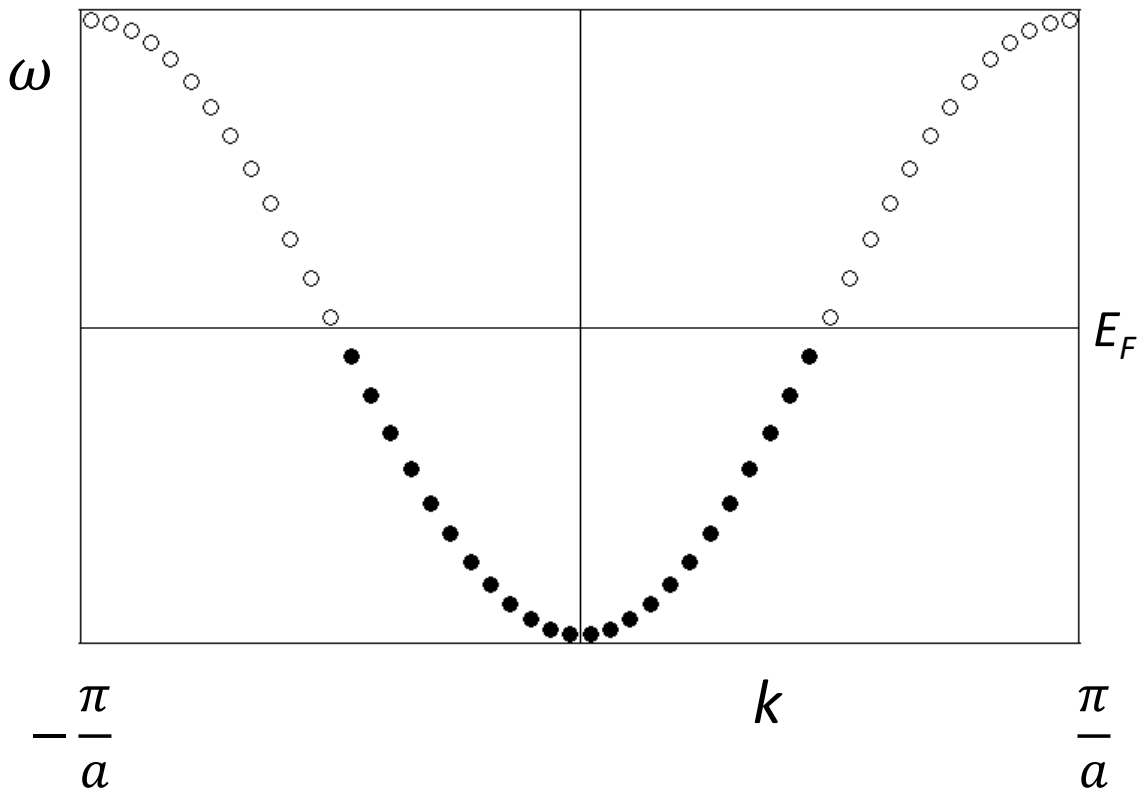
z = -cos(2*pi*x/2)-0.2*cos(2*pi*y/2

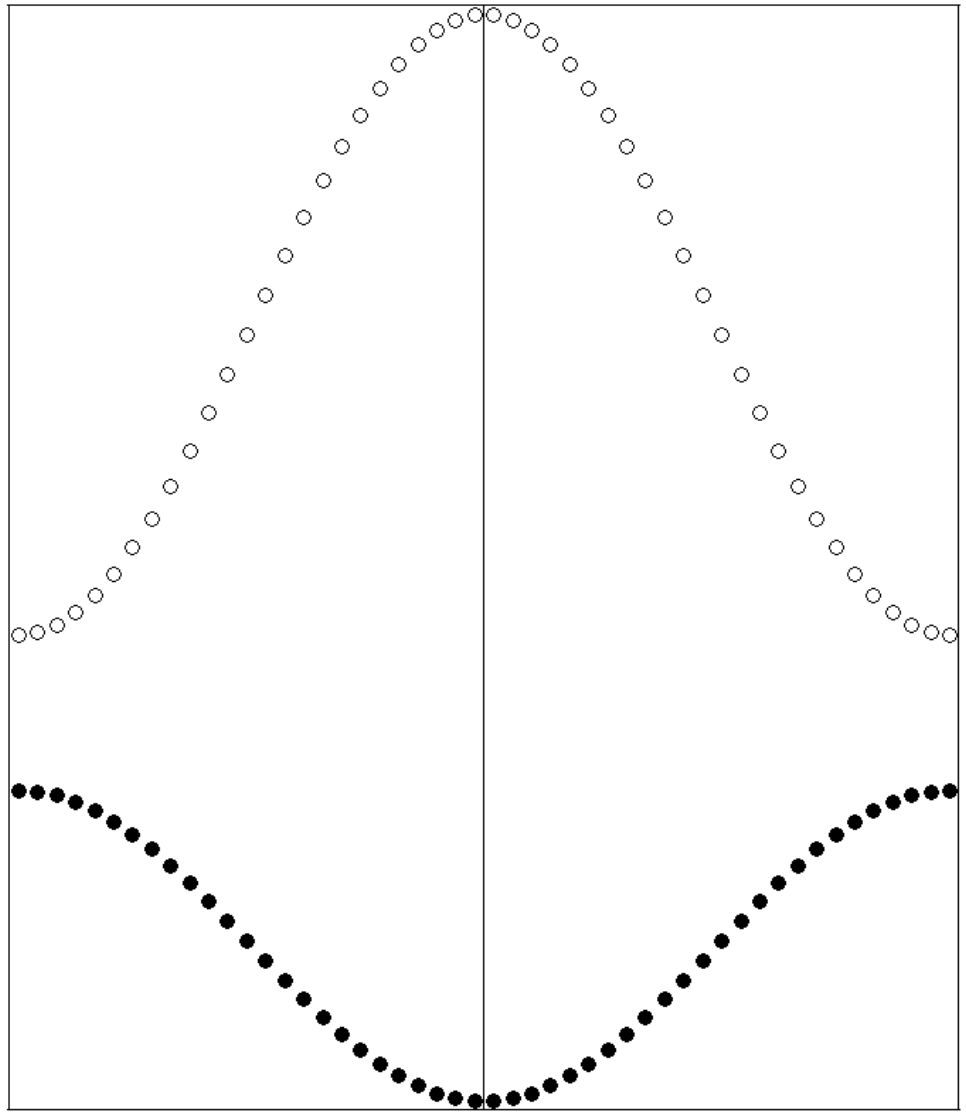
Number of Gridlines 30

Електронна зонна структура

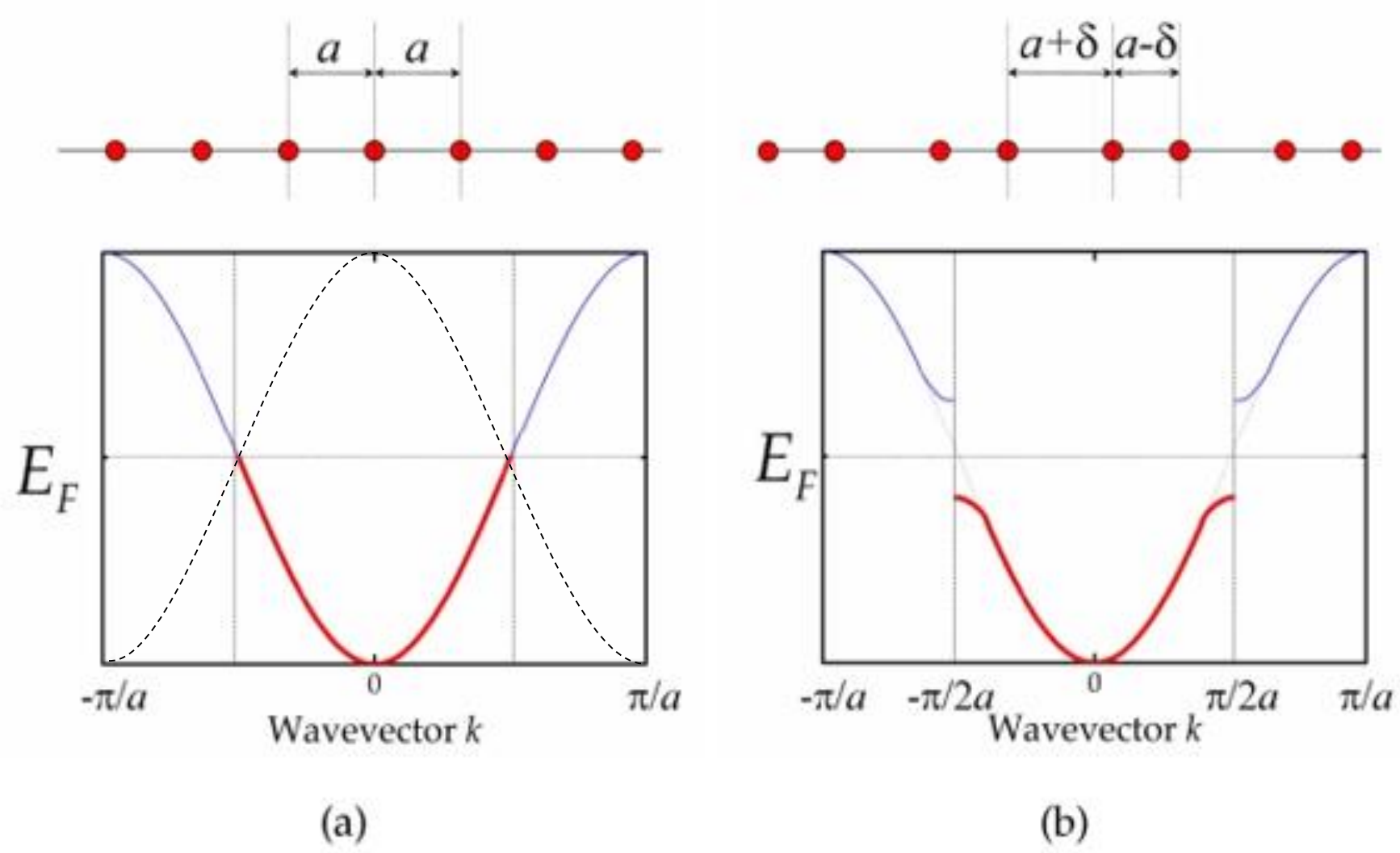


Metal *vs* Insulator

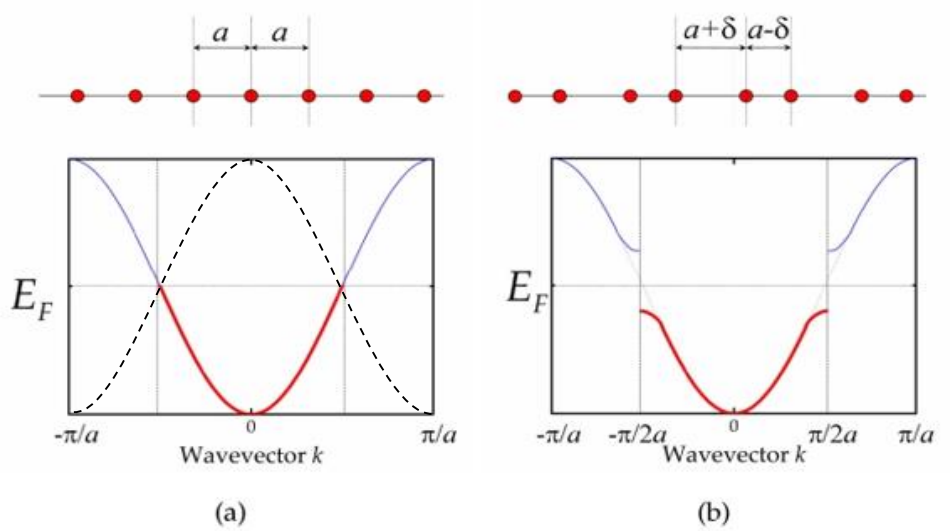


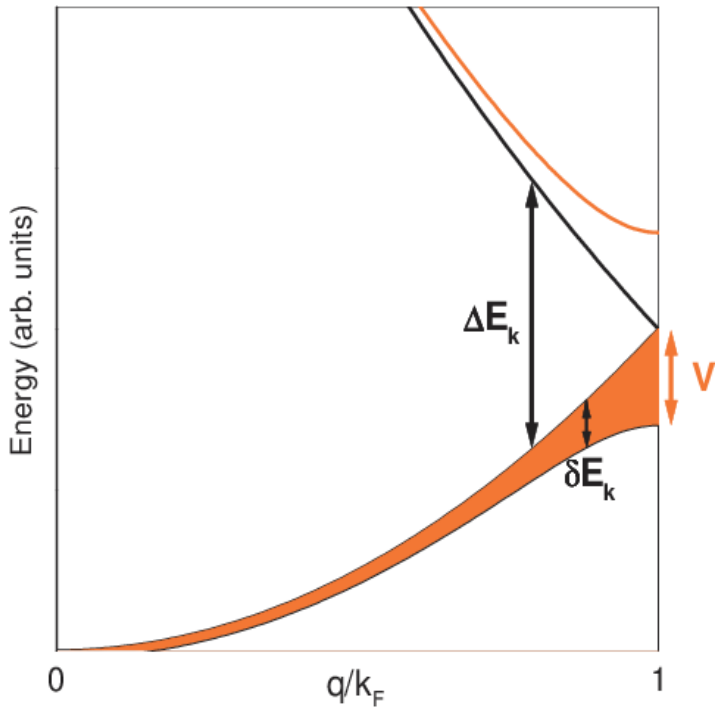


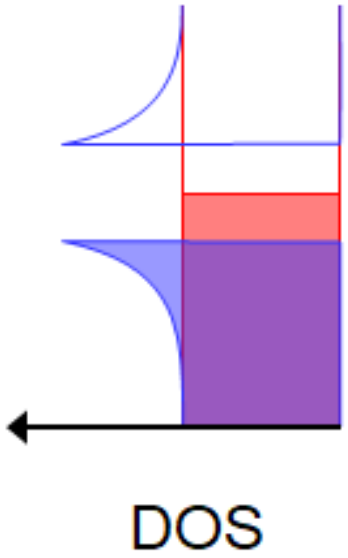
Peierls transition and Fermi surface nesting



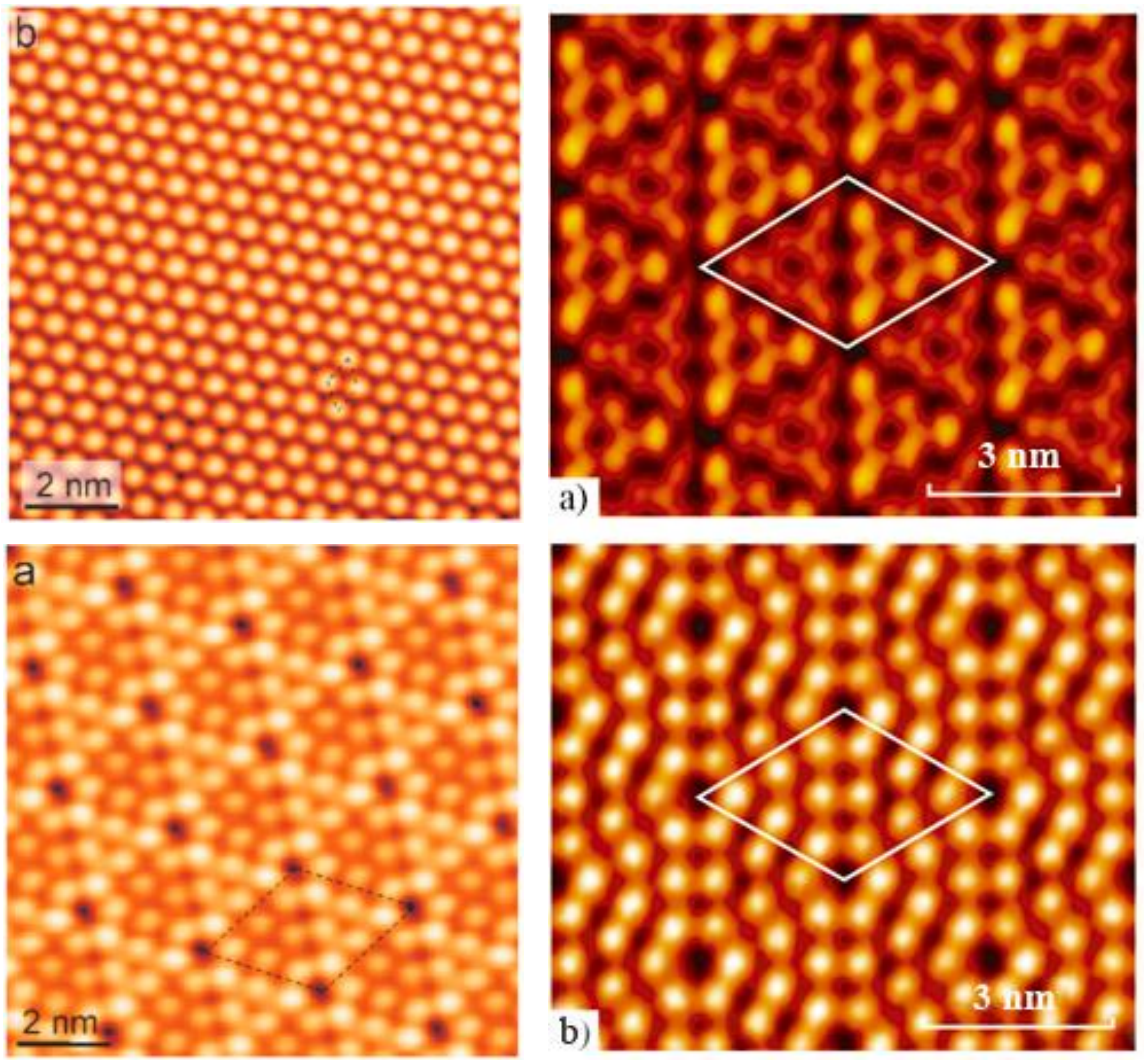
Peierls transition and Fermi surface nesting

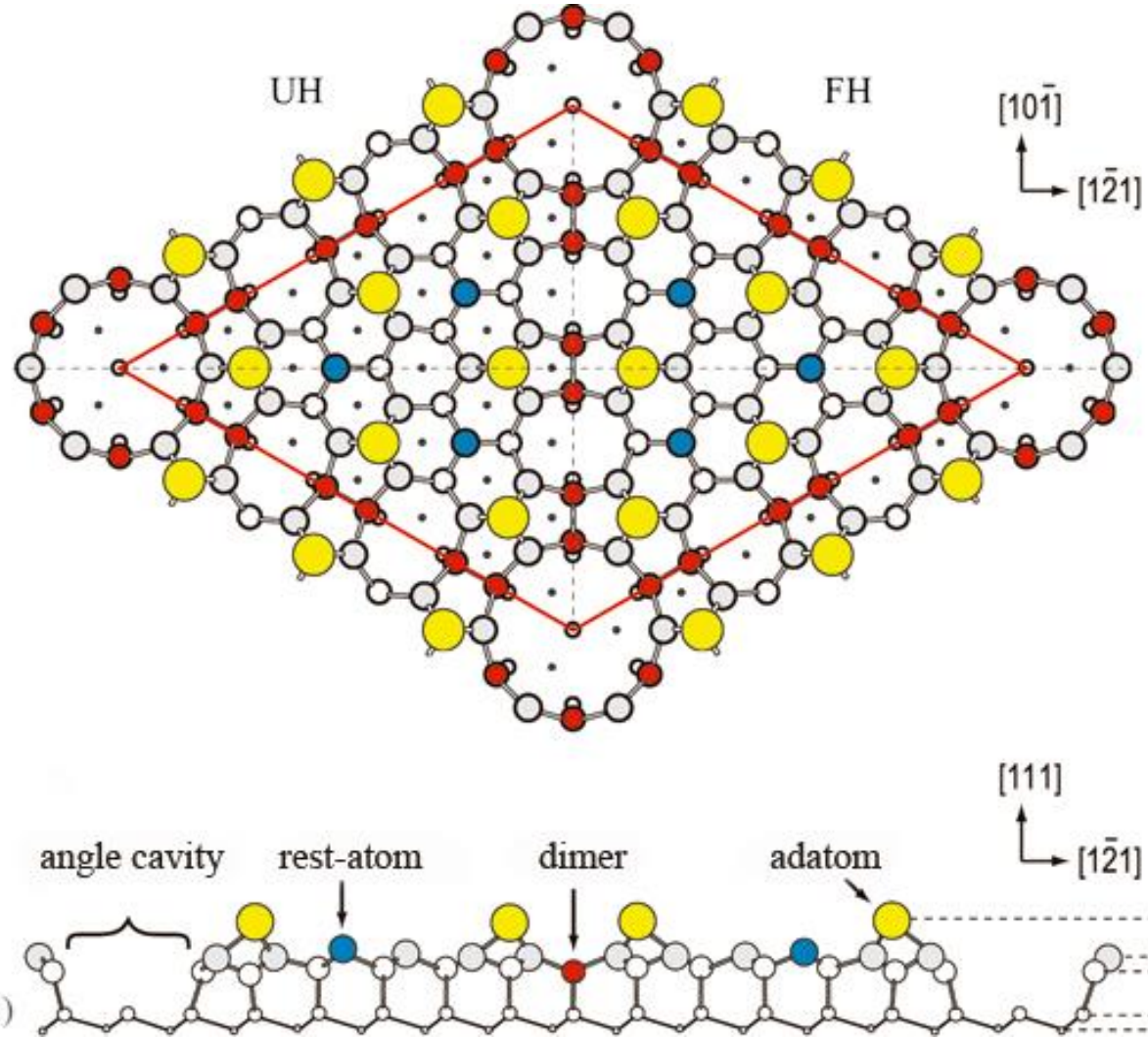






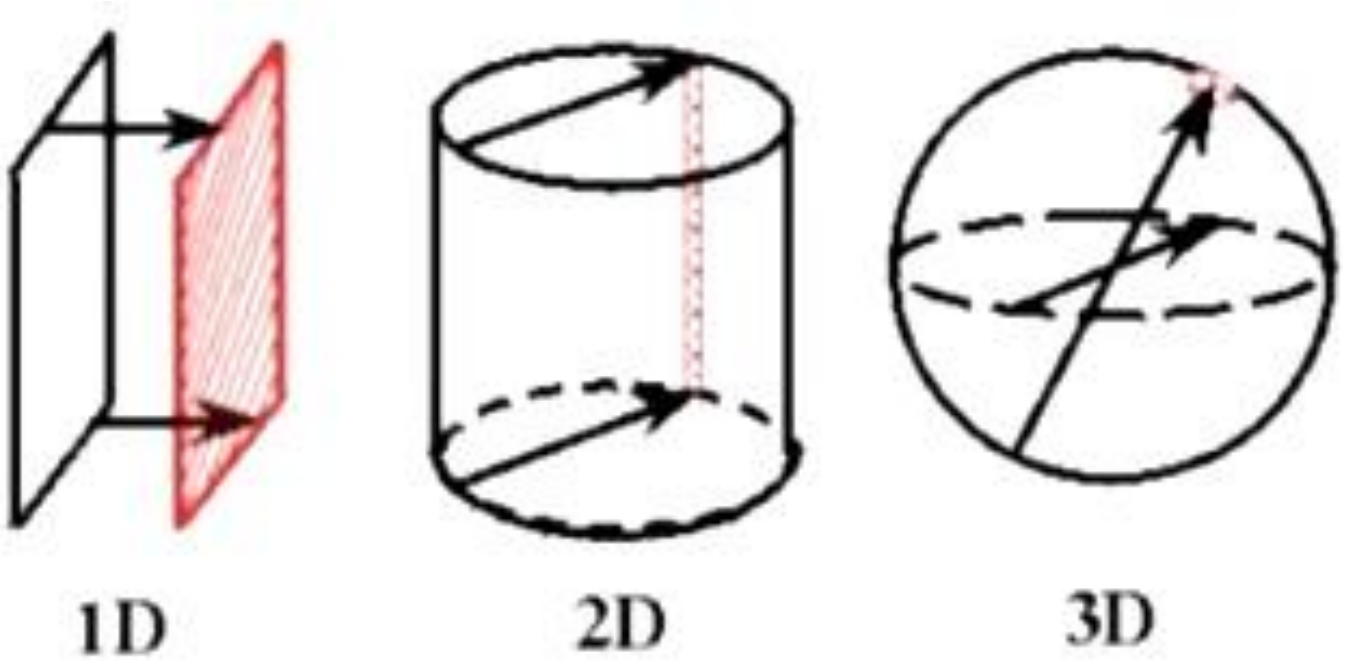
7×7 surface reconstruction of Si(111)



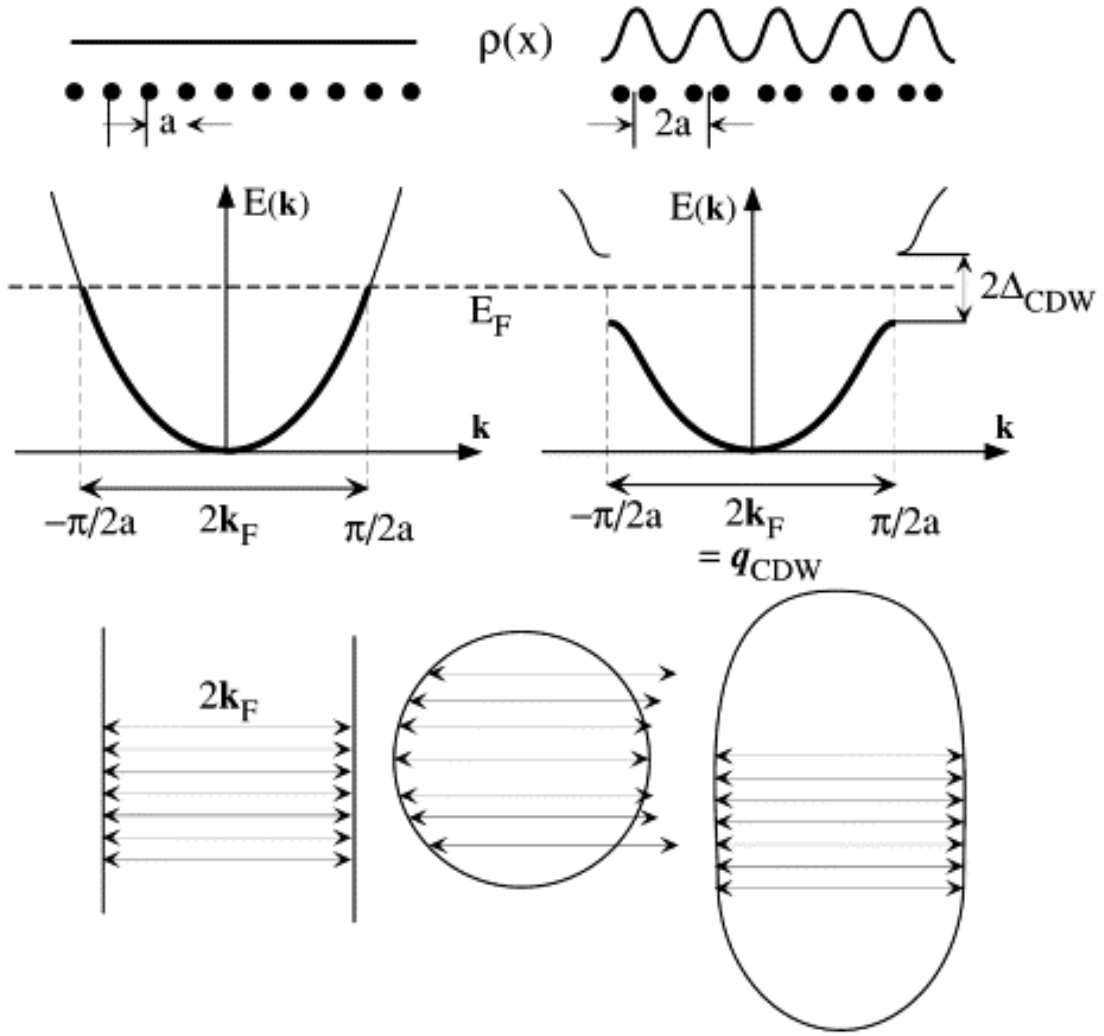


K. Takayanagi *Surf. Sci.* 164, 367 (1985)

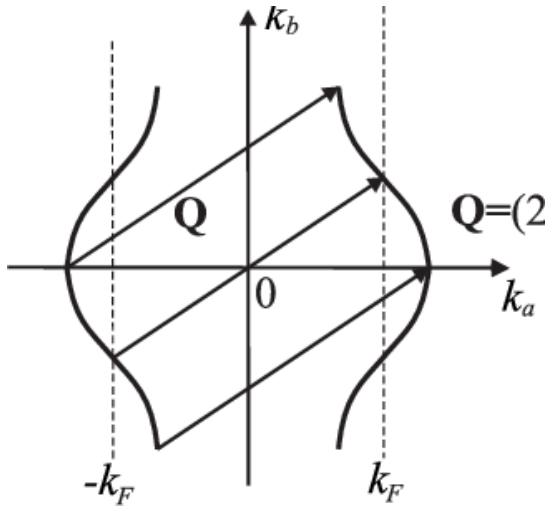
Peierls transition and Fermi surface nesting

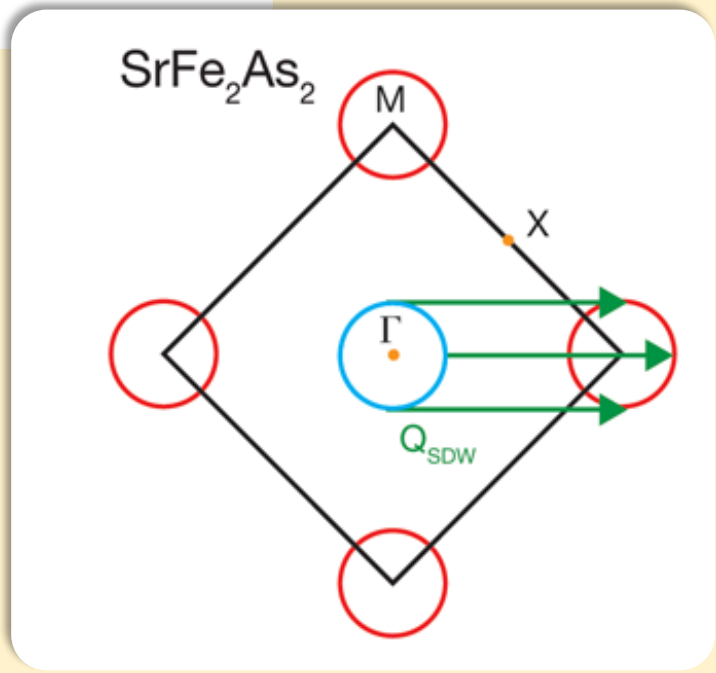


Peierls transition and Fermi surface nesting

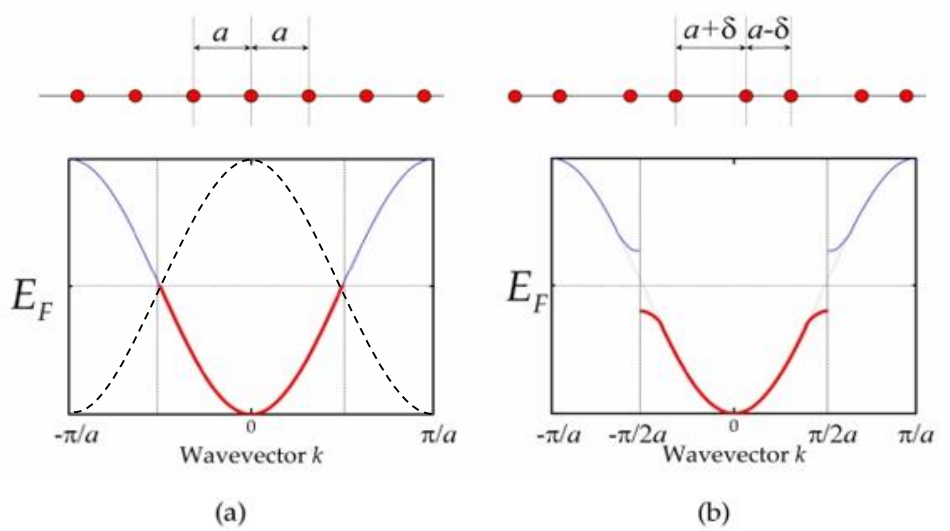


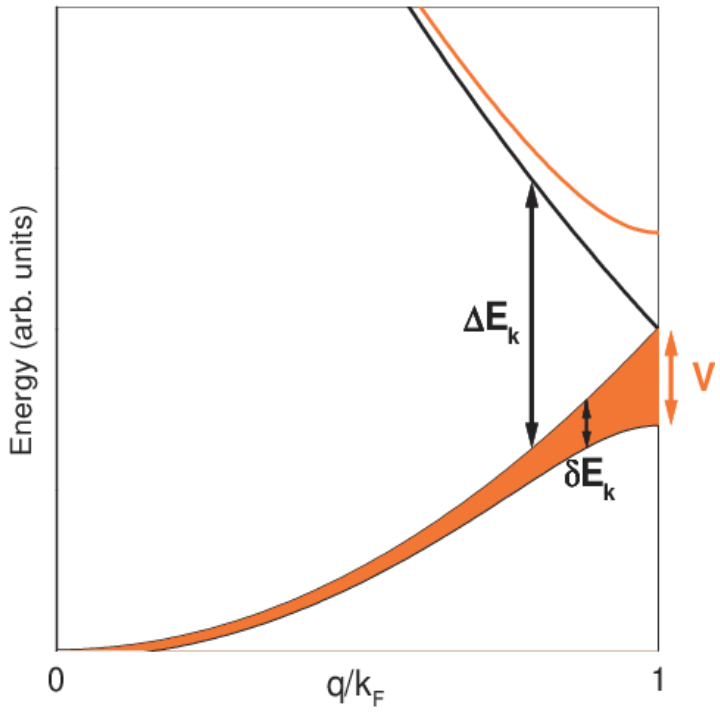
Aebi *JESRP* 2001 https://doi.org/10.1016/S0368-2048(01)00262-6

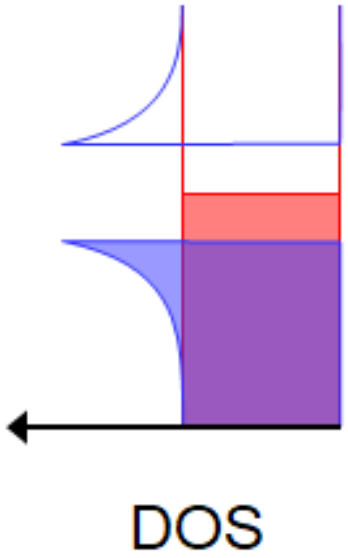


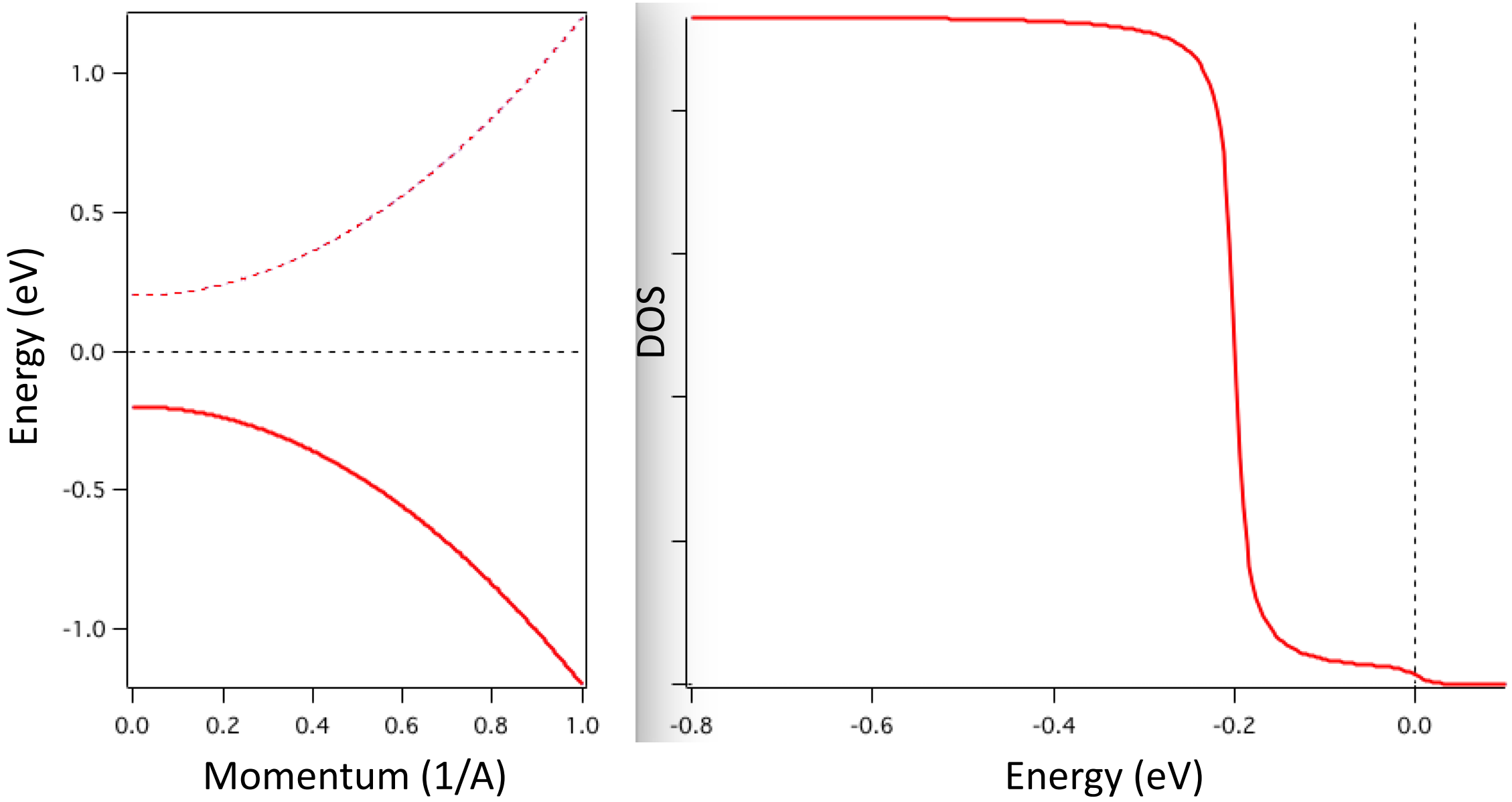


Peierls transition and Fermi surface nesting

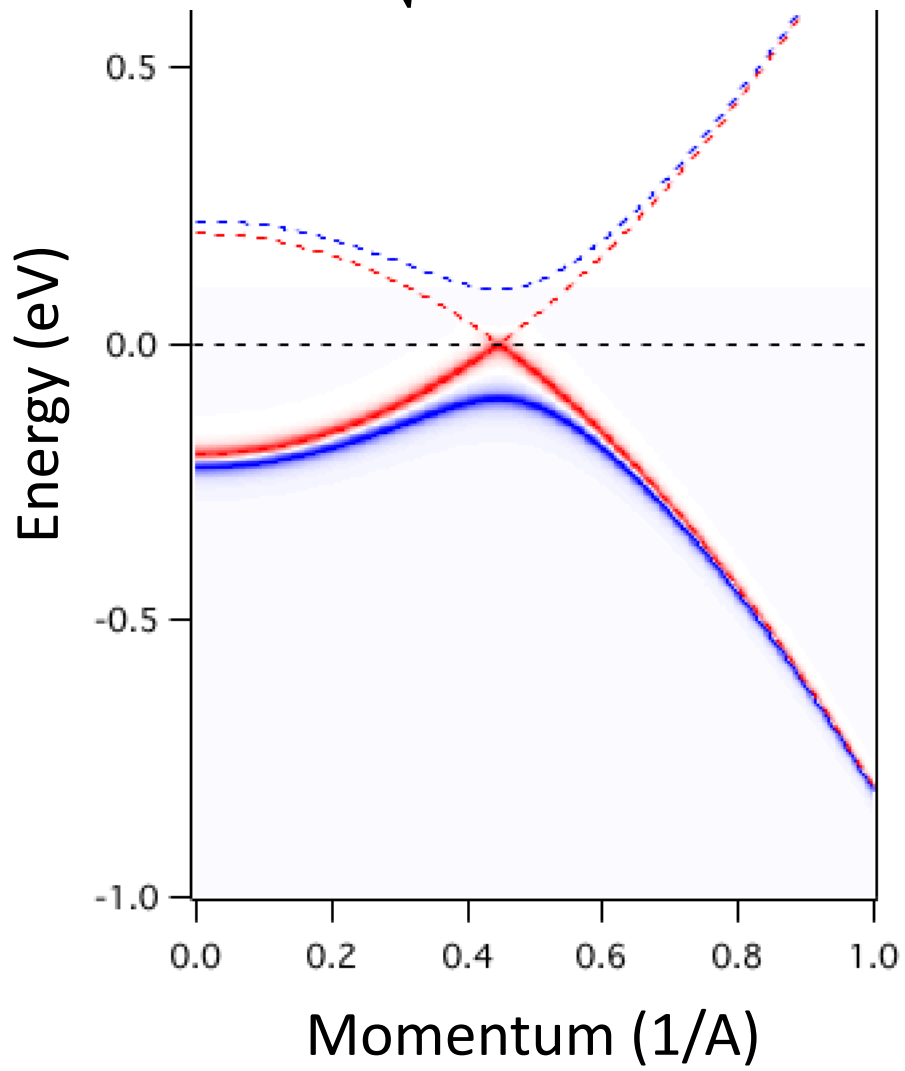


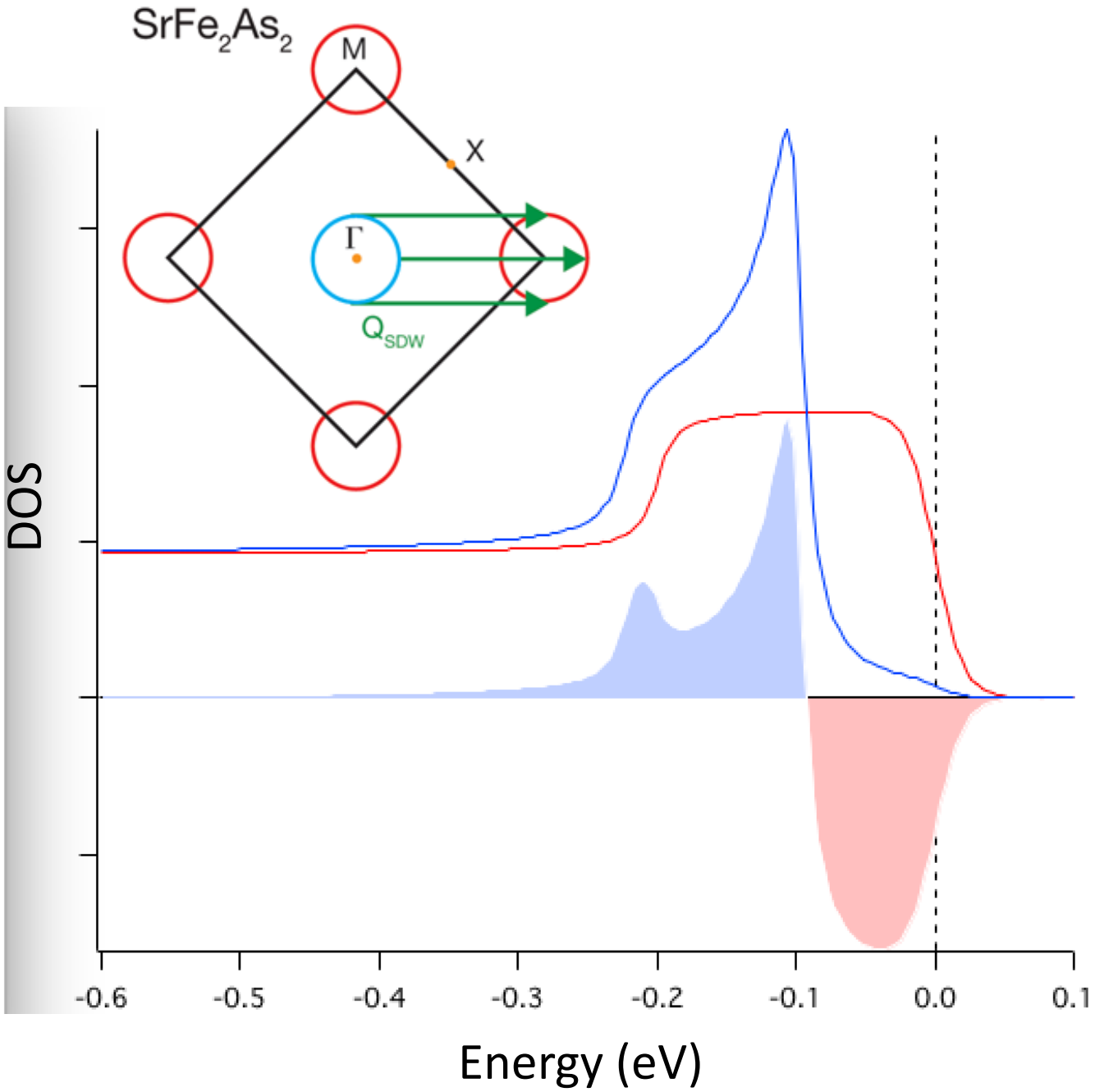


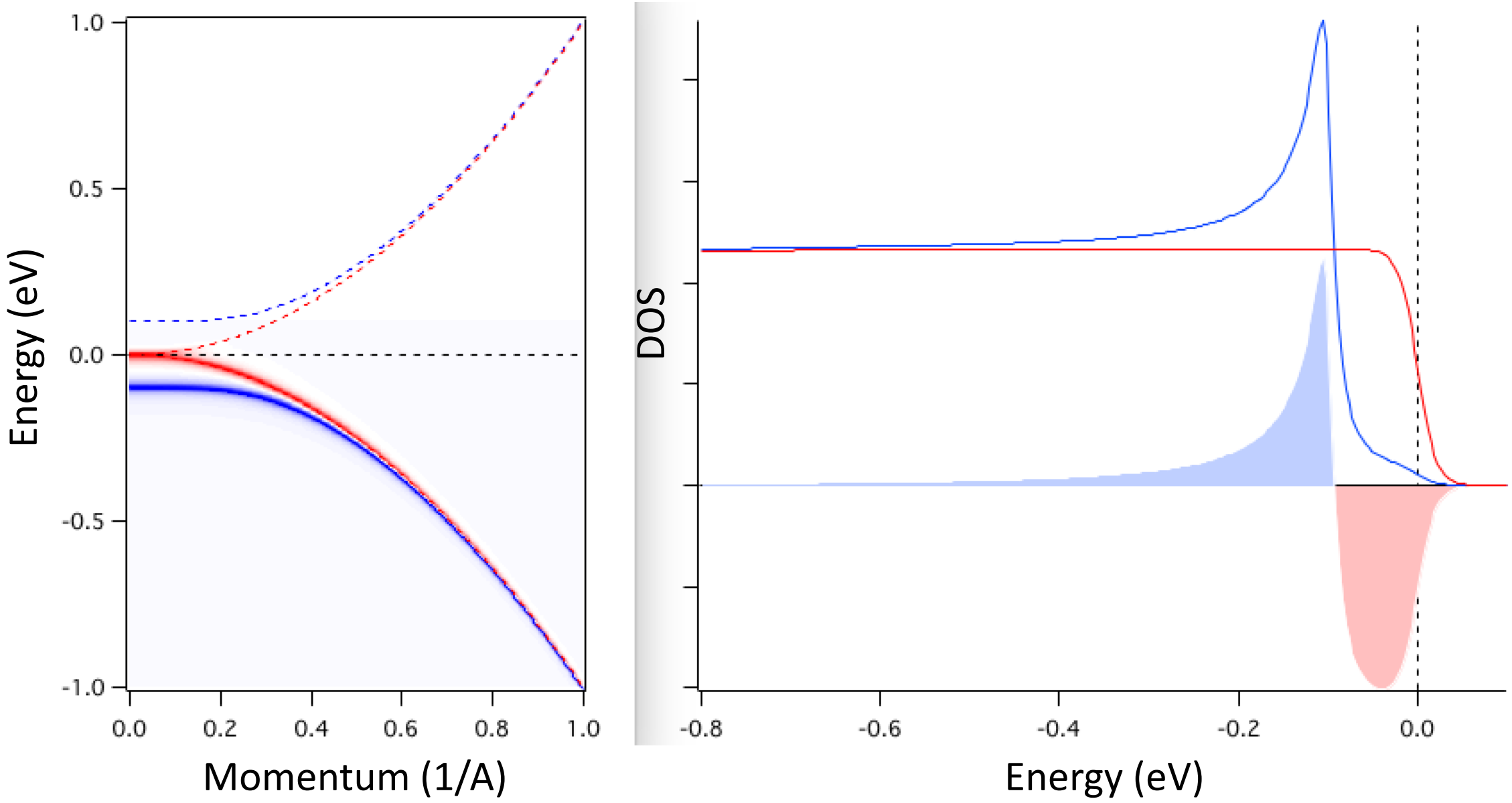


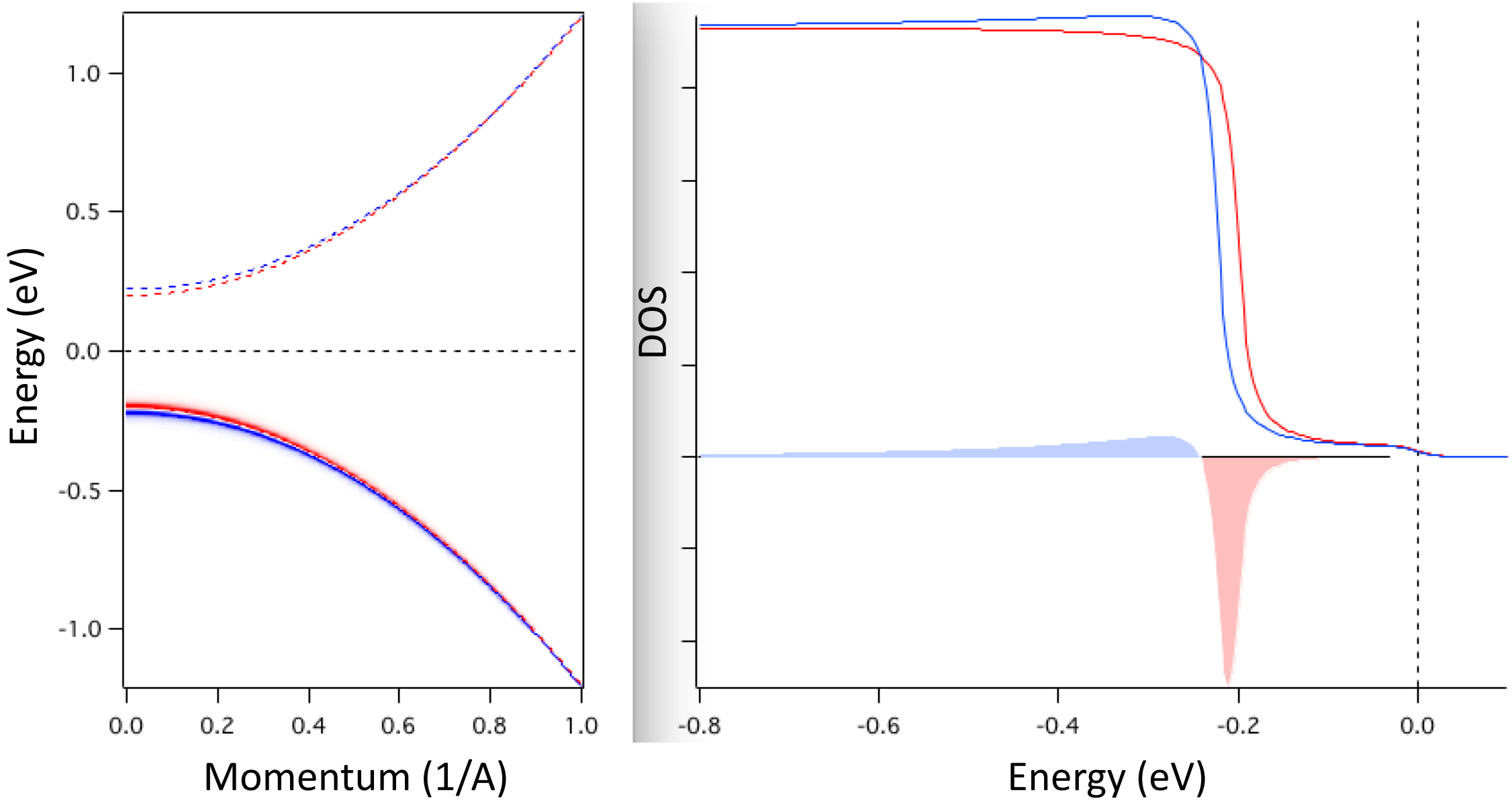

1.0
0.5
0.0
-0.5
-1.0
Energy (eV)
0.0
0.2
0.4
0.6
0.8
1.0
Momentum (1/A)
DOS
-0.8
-0.6
-0.4
-0.2
0.0
Energy (eV)

$$\varepsilon_{\pm} = \frac{\varepsilon_1+\varepsilon_2}{2} \pm \sqrt{\left(\frac{\varepsilon_1-\varepsilon_2}{2}\right)^2 + \Delta^2}$$






1.0
0.5
0.0
-0.5
-1.0
Energy (eV)
0.0
0.2
0.4
0.6
0.8
1.0
Momentum (1/A)
DOS
-0.8
-0.6
-0.4
-0.2
0.0
Energy (eV)


1.0
0.5
0.0
-0.5
-1.0
Energy (eV)
0.0
0.2
0.4
0.6
0.8
1.0
Momentum (1/A)
DOS
-0.8
-0.6
-0.4
-0.2
0.0
Energy (eV)

Developed with support from NSF-IUSE #1524968.

E

F

Graph | 3D Mode

x = 1.963

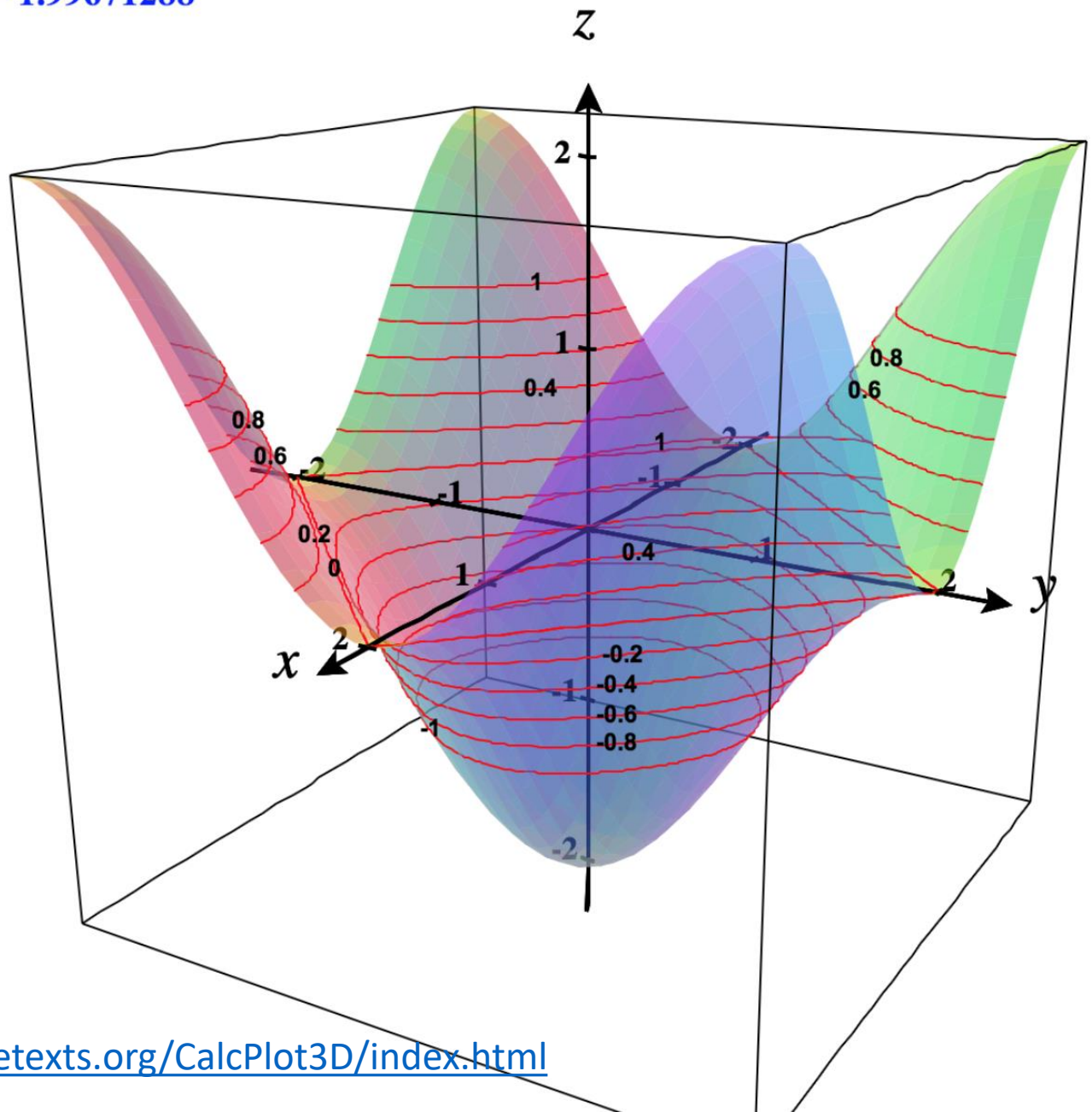
y = 1.963

Add to graph: Select...

z = -cos(pi*x/2)-cos(pi*y/2)

Number of Gridlines 30

$f(1.9635, 1.9635) = 1.99671288$



https://c3d.libretexts.org/CalcPlot3D/index.html

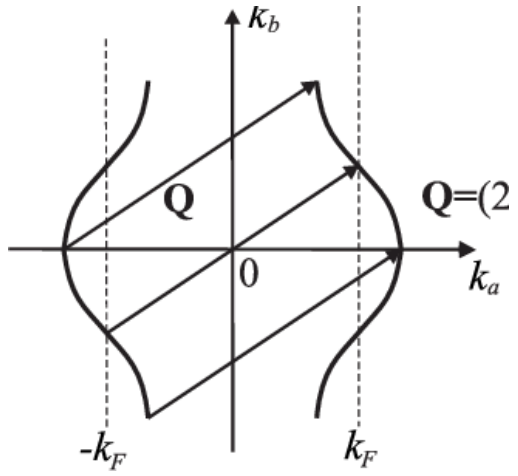
Developed with support from NSF-IUSE #1524968.

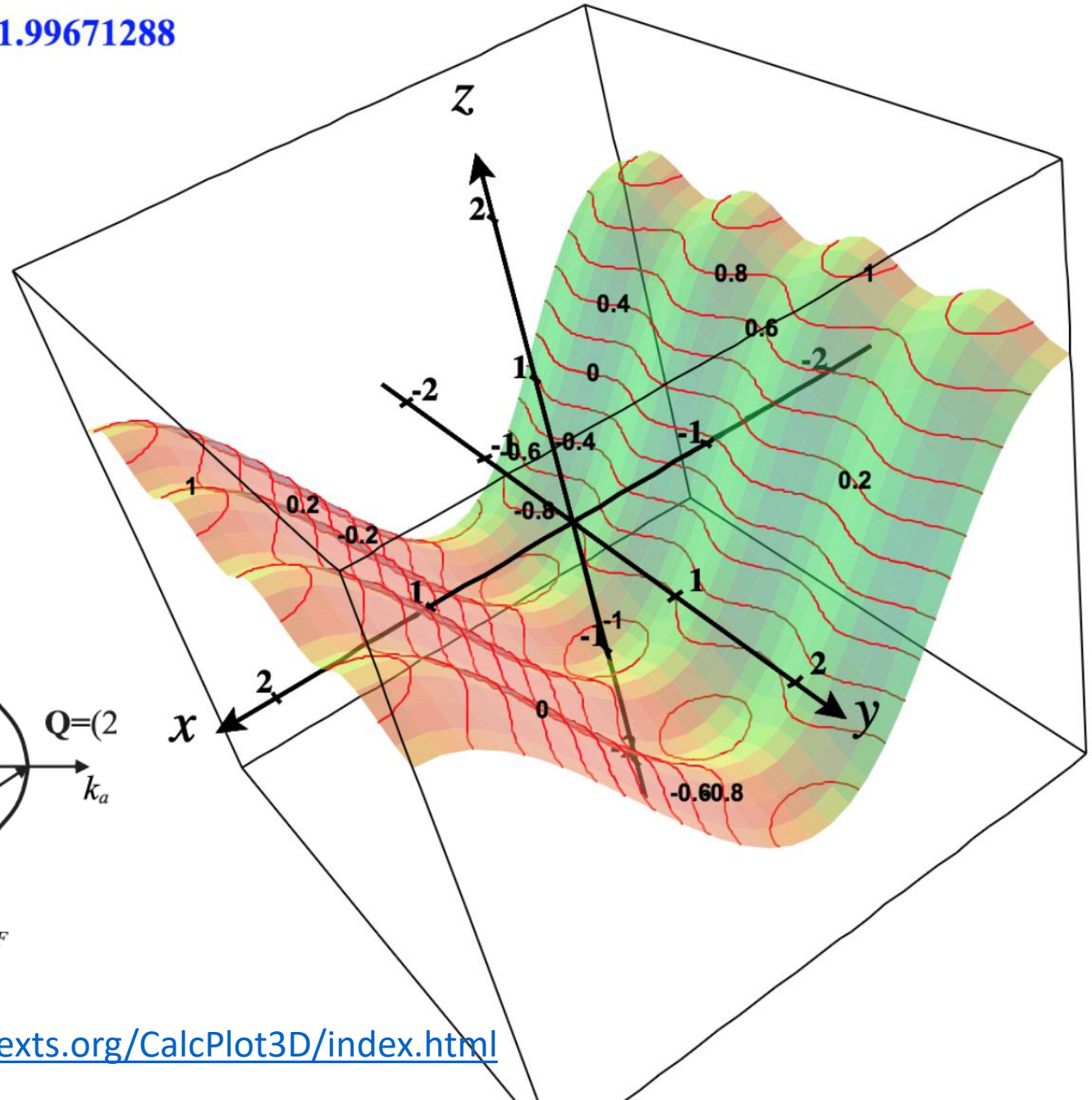
E

F

Graph | 3D Mode

$f(1.9635, 1.9635) = 1.99671288$





$x =$ 1.963

$y =$ 1.963

Add to graph: Select...

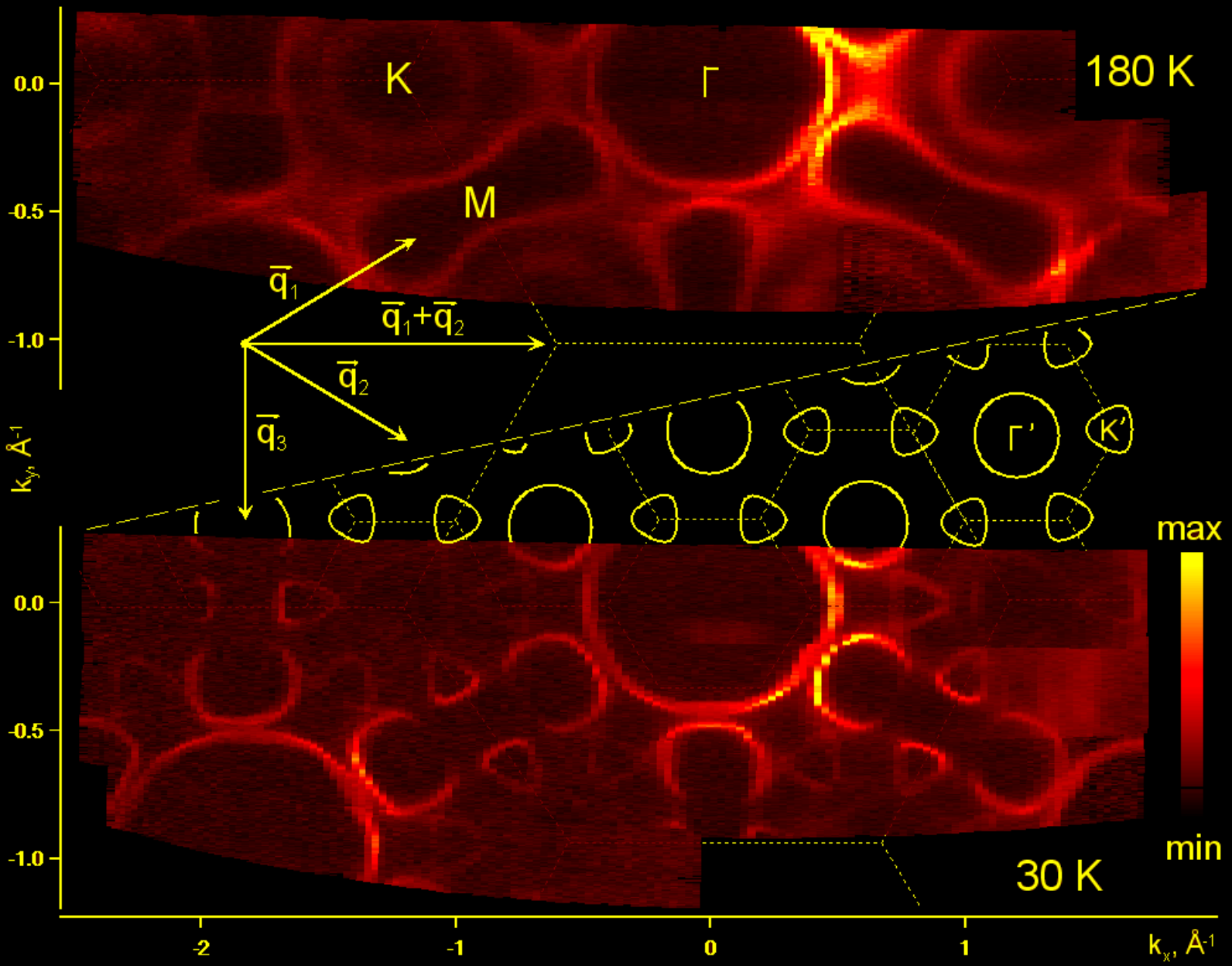
z = -cos(pi*x/2)-0.1*cos(4*pi*y/2)

Number of Gridlines 30

https://c3d.libretexts.org/CalcPlot3D/index.html

У наступній лекції: Хвилі зарядової густини в дихалькогенідах перехідних металів

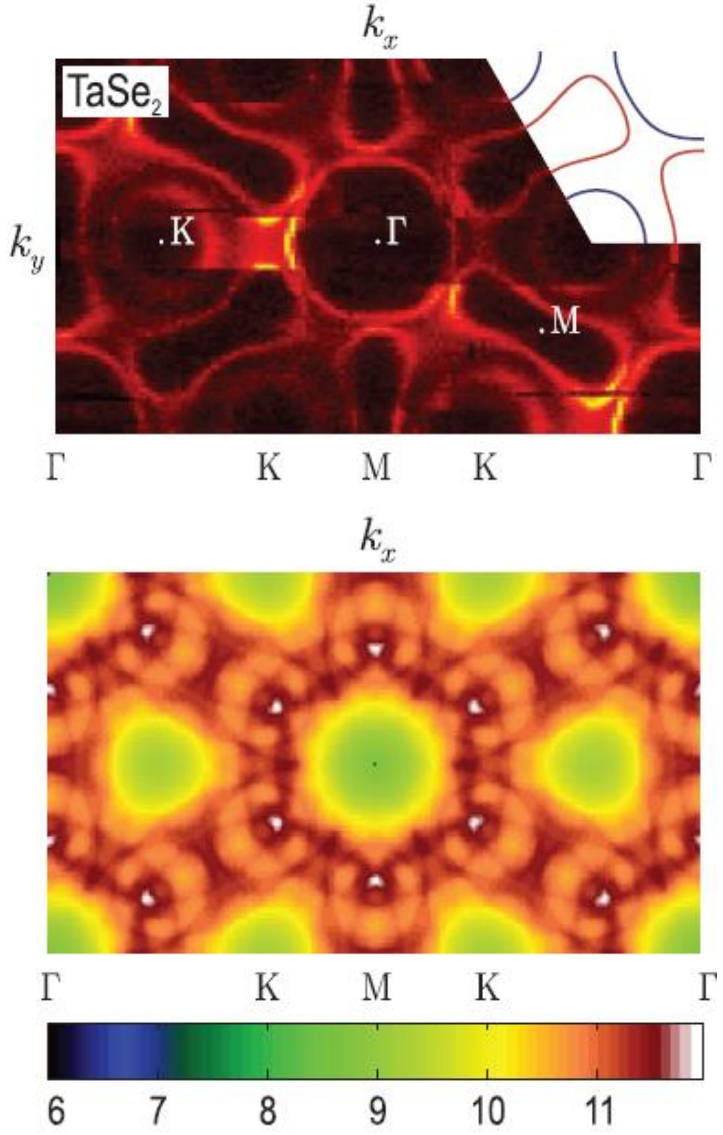
CDW in $TaSe_2$



Borisenko *PRL* 2008

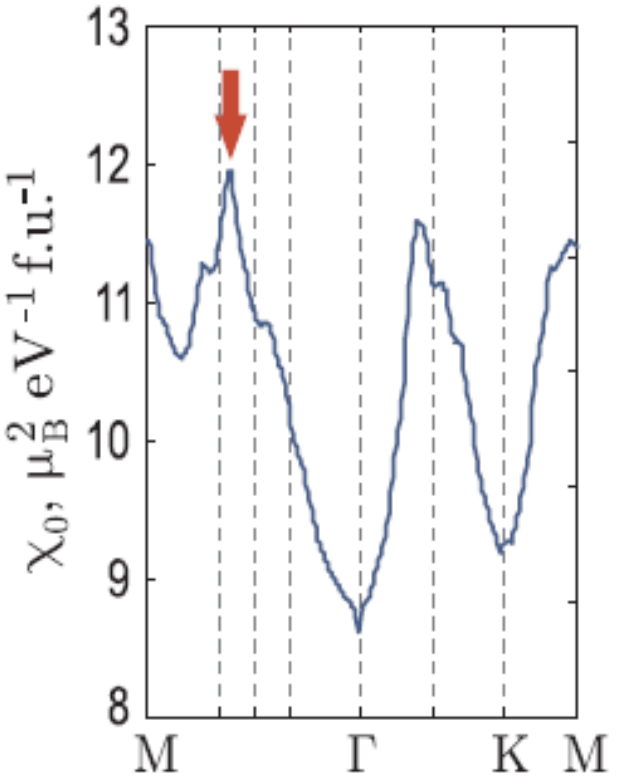
У наступній лекції:

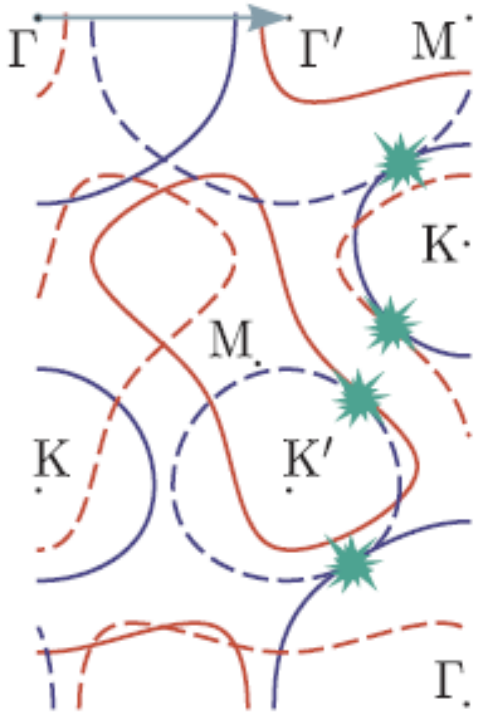
Fermi surface nesting



$$\chi_{\mathbf{q}} = \sum_{\mathbf{k}} [n_F(\epsilon_{\mathbf{k}}) - n_F(\epsilon_{\mathbf{k+q}})]/(\epsilon_{\mathbf{k}} - \epsilon_{\mathbf{k+q}})$$

$$\chi = G \star G$$





Inosov *NJP* 2008