

Miller Indices

$$h_{wv} := \text{floor}\left(\frac{wv + 62}{Gsz^2}\right) - FG \quad k_{wv} := \text{floor}\left(\frac{\text{mod}(wv + 62, Gsz^2)}{Gsz}\right) - FG \quad l_{wv} := \text{mod}(wv + 62, Gsz) - FG$$

D:

Reciprocal Vector

$$K_{wv} := h_{wv} \cdot b1 + k_{wv} \cdot b2 + l_{wv} \cdot b3$$

Dimensionless
Vector Module

$$Mdl_{wv} := \text{round}\left[\left(\frac{ao}{2 \cdot \pi}\right)^2 \cdot K_{wv} \cdot K_{wv}\right]$$

Form Factors

$$Vs_{124} := 0 \quad Vs_{wv} := \begin{cases} VS3 \cdot Ry & \text{if } Mdl_{wv} = 3 \\ VS8 \cdot Ry & \text{if } Mdl_{wv} = 8 \\ VS11 \cdot Ry & \text{if } Mdl_{wv} = 11 \\ 0 & \text{otherwise} \end{cases}$$

Hamiltonian indices

$$ORIGIN := -62 \quad i := -62..62 \quad j := -62..62 \quad (\text{Shift column vector Vs and K rank by +62})$$

Matrix Element Γ

$$H\Gamma_{i,j} := \lambda eV \cdot \left(|\Gamma_v + K_{i+62}| \right)^2 \cdot \delta(i,j) + Vs_{i-j+62} \cdot \cos(K_{i-j+62} \cdot \tau)$$

Γ point Eigenvalues

$$E_\Gamma := \text{sort}(\text{Re}(\text{eigenvals}(H\Gamma)))$$

$$E_\Gamma^T =$$

	-62	-61	-60	-59	-58	-57	-56
-62	-2.155	10.483	10.485	10.548	13.858	13.878	13.895

$$\text{length}(E_\Gamma) = 125$$

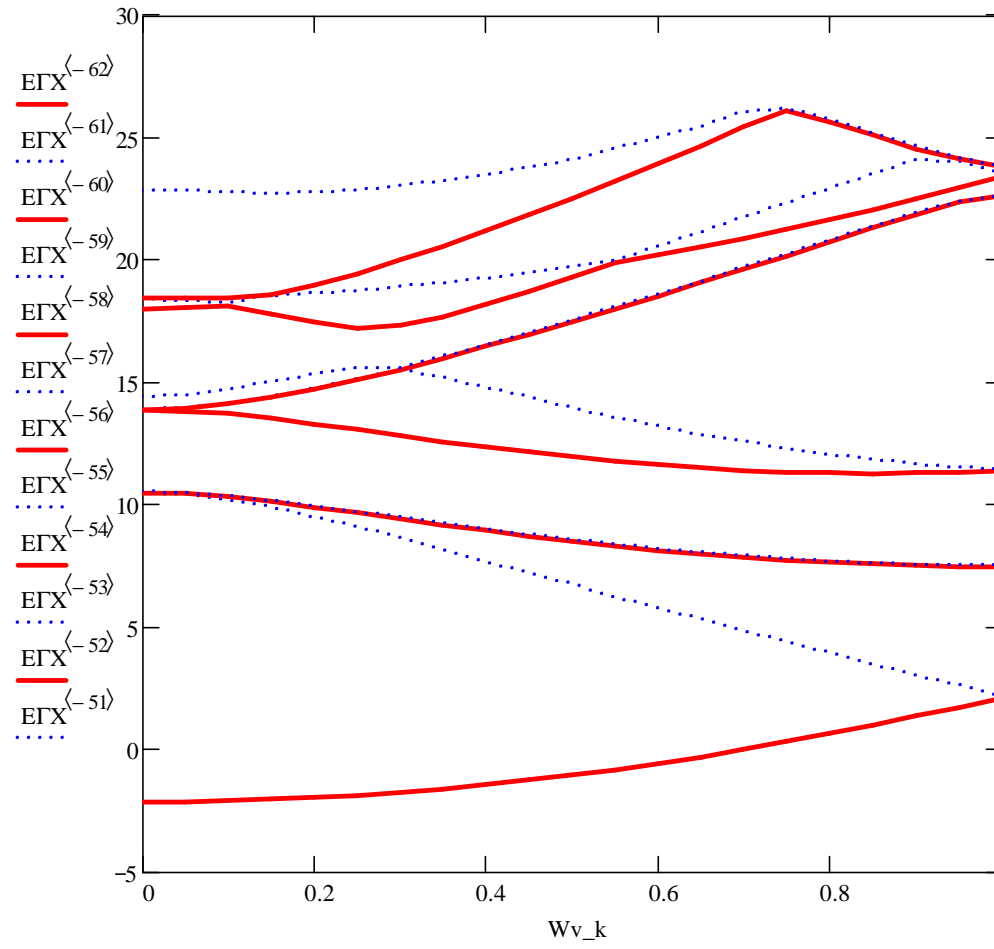
$\Gamma - X$

$$E\Gamma X := \begin{cases} \text{for } It_1 \in 0..20 \\ \quad WvR \leftarrow \frac{2\pi}{ao} \begin{pmatrix} \frac{It_1}{20} \\ 0 \\ 0 \end{pmatrix} \\ \quad \text{for } i \in -62..62 \\ \quad \quad \text{for } j \in -62..62 \\ \quad \quad \quad H\Gamma X_{i,j} \leftarrow \lambda eV \cdot \left(|WvR + K_{i+62}| \right)^2 \cdot \delta(i,j) + Vs_{i-j+62} \cdot \cos(K_{i-j+62} \cdot \tau) \\ \quad \quad \quad \text{Buffer}_1 \leftarrow \text{sort}(\text{Re}(\text{eigenvals}(H\Gamma X))) \\ \quad \quad \quad \text{for } It_2 \in -62..62 \\ \quad \quad \quad \quad \text{Buffer}_2 \text{ORIGIN} + It_1, It_2 \leftarrow \text{Buffer}_1 It_2 \\ \quad \text{Buffer}_2 \end{cases}$$

Coordinate axis index

$It_1 := 0..20$

$$Wv_kORIGIN+It_1 := \frac{It_1}{20}$$



Comments

Function Round mandatory for Mdl variable. Otherwise Mathcad (13) misses integer value 11 during from factor sorting.

If variable wv not specified as an integer ($wv := -124..124$), Mathcad (13) plots non integer values larger than 2 for $l(wv)$ plot.

Mathcad manages Matrices with all indexes starting at same origin (i.e. either -124 or -62)

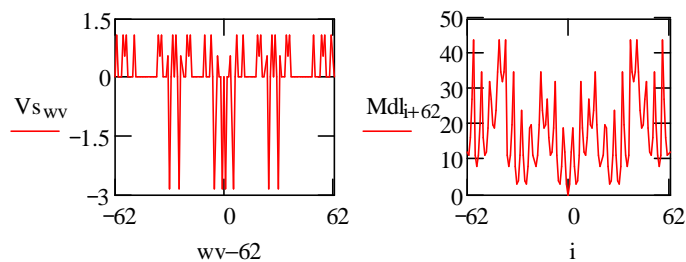
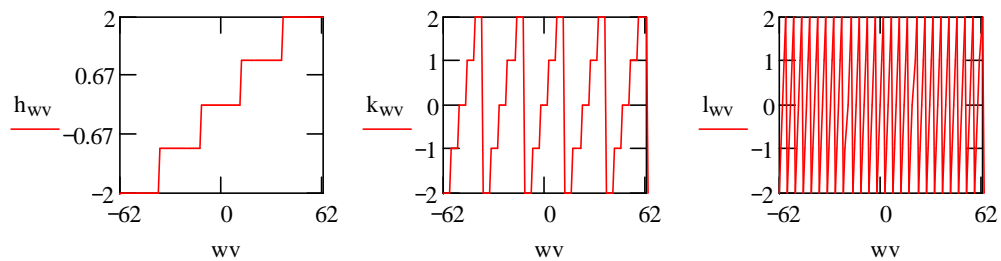
Acknowledgements

h, k, l computation algorithm taken from A. Danner's Mathematica program.

<http://www.ece.nus.edu.sg/stfpage/eleadj/pseudopotential.htm> Last accessed 10/09/2007

Eigenvalue calculation loop from Stevens aln (Mathcad users forum).

ata check



$$PE_{i,j} := V_{s_{i-j+62}} \cdot \cos(K_{i-j+62} \cdot \tau)$$

$H\Gamma =$

	-62	-61
-62	61.145	-2.02
-61	-2.02	56.05
-60	0	-2.02
-59	0	0
-58	0.544	0
-57	-2.02	0.544

