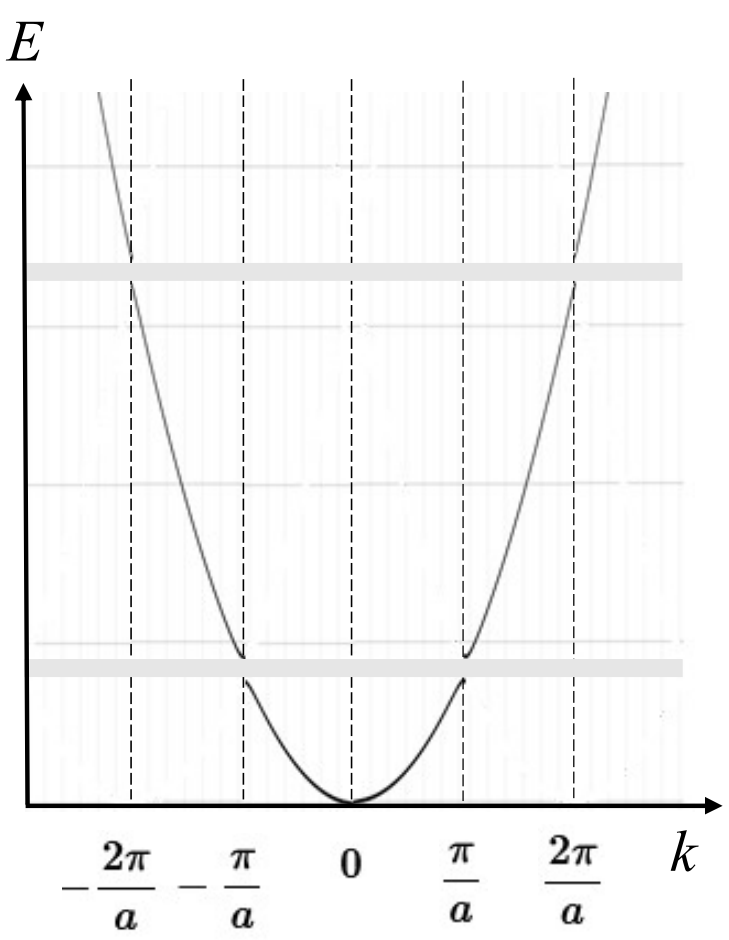
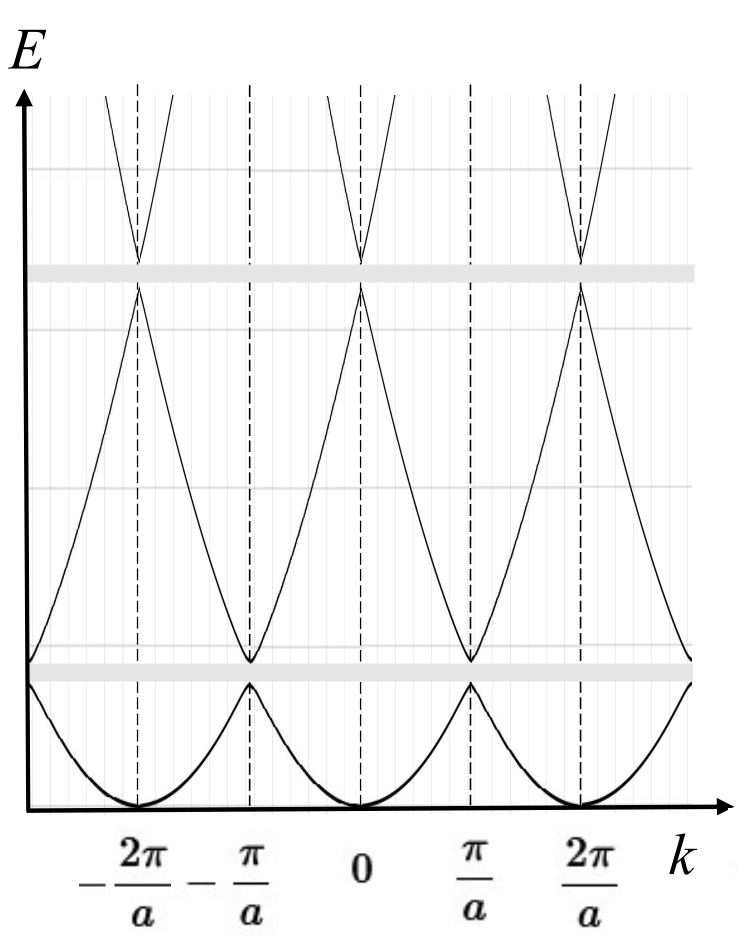
Electron Band Structure

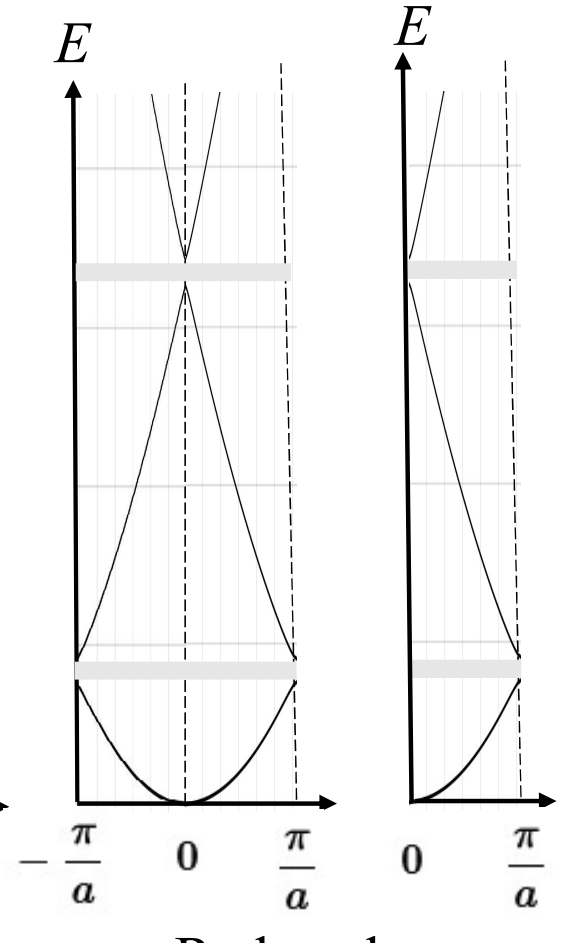
Empty lattice approximation



Extended



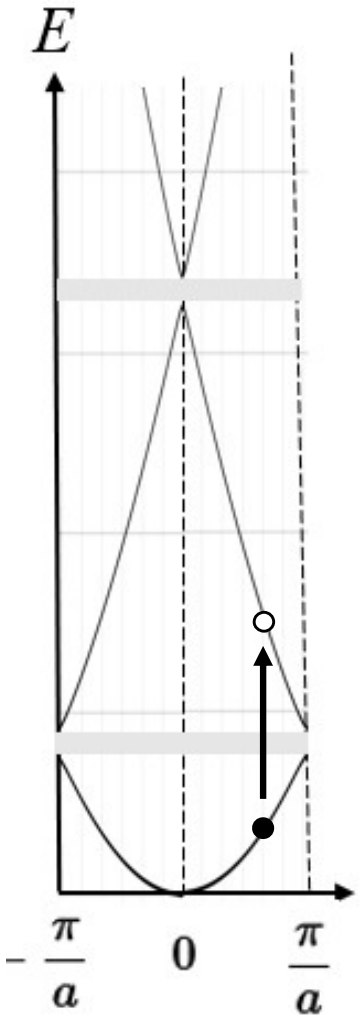
Repeated



Reduced

$$\psi_{\vec{k}}(\vec{r}) = e^{i\vec{k}\cdot\vec{r}} \sum_{\vec{G}} C_{\vec{G}} e^{i\vec{G}\cdot\vec{r}} = e^{i\vec{k}\cdot\vec{r}} \underbrace{e^{i\vec{G}_0\cdot\vec{r}} e^{-i\vec{G}_0\cdot\vec{r}}}_{1} \sum_{\vec{G}} C_{\vec{G}} e^{i\vec{G}\cdot\vec{r}} = e^{i\left(\vec{k}-\vec{G}_0\right)\cdot\vec{r}} \sum_{\vec{G}} C_{\vec{G}} e^{i\left(\vec{G}+\vec{G}_0\right)\cdot\vec{r}}$$

Conservation of momentum

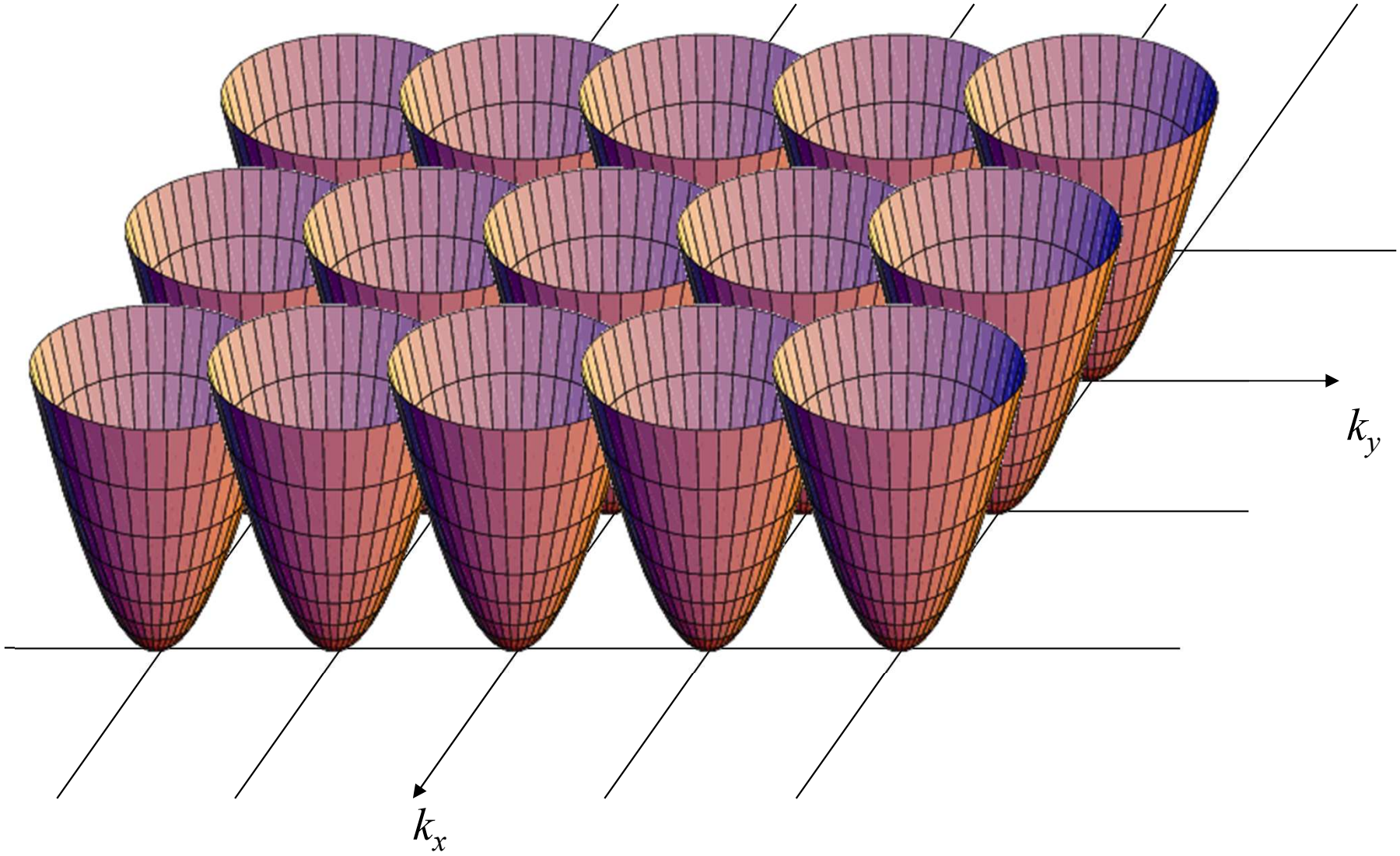


When an electron absorbs a photon and makes a transition from an occupied state to an empty state, energy and momentum are conserved.

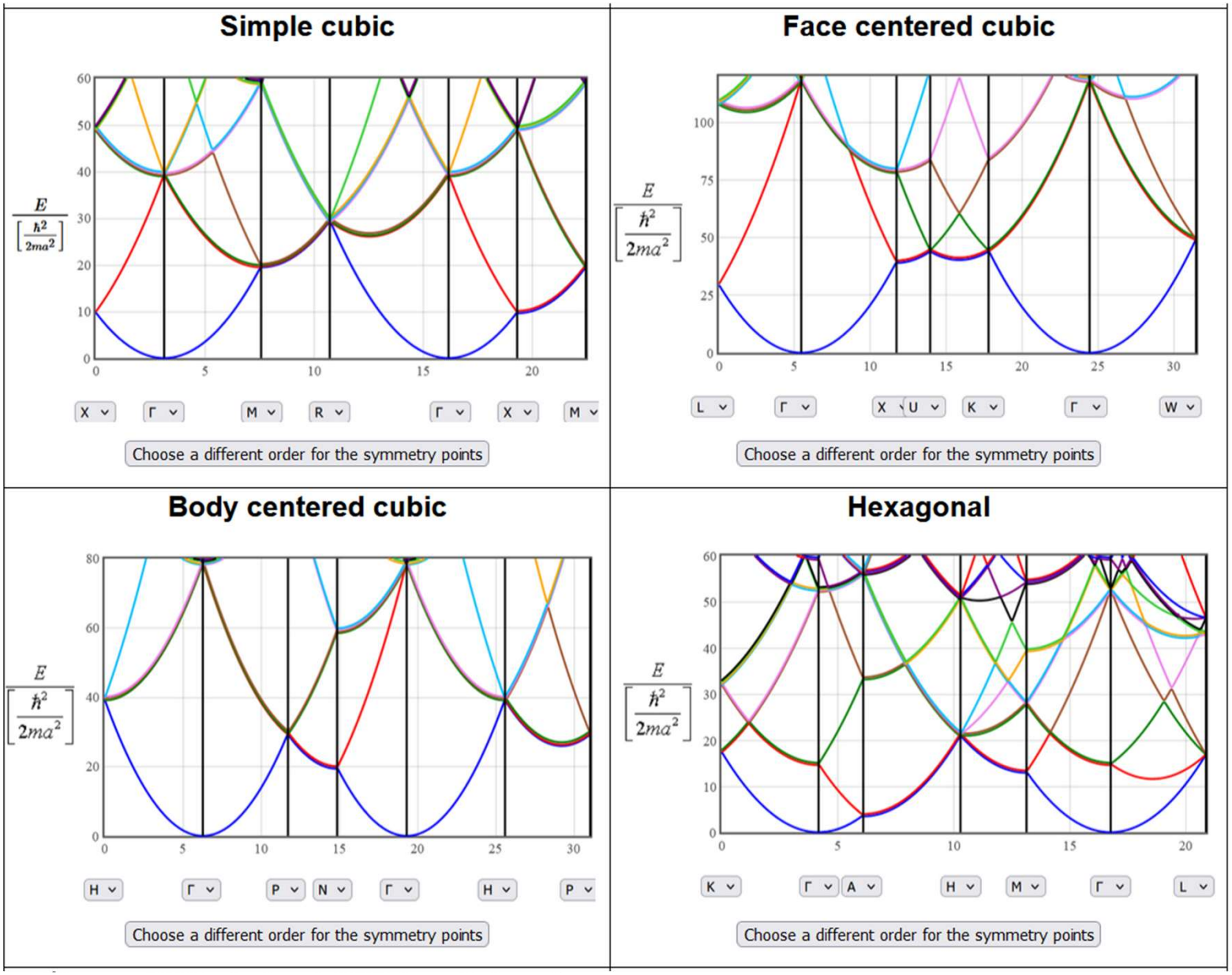
$$\hbar\vec{k}_{\text{photon}} + \hbar\vec{k}_{\text{initial}} = \hbar\vec{k}_{\text{final}} + \hbar\vec{G}$$

$$\vec{k}_{\text{initial}} = \vec{k}_{\text{final}} + \vec{G}$$

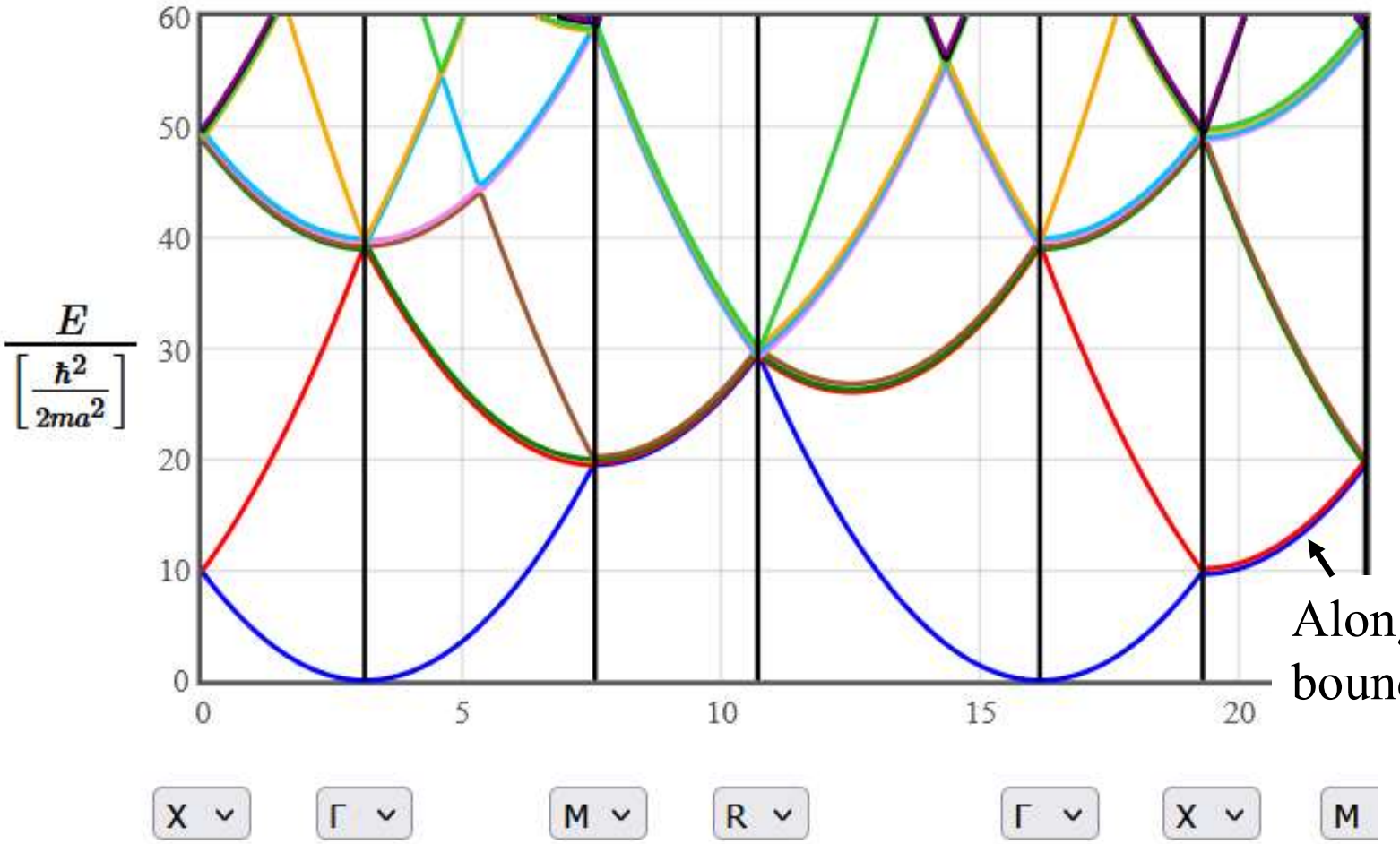
Empty lattice approximation



Empty lattice approximation



Empty lattice approximation



Along the BZ boundary

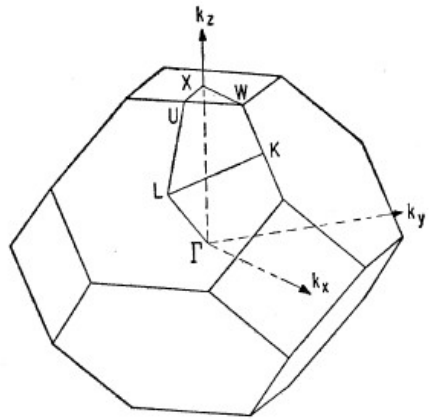
There are as many *k* states per band as there are primitive unit cells in the crystal.

There are 2 electrons states (spin) per *k* state.

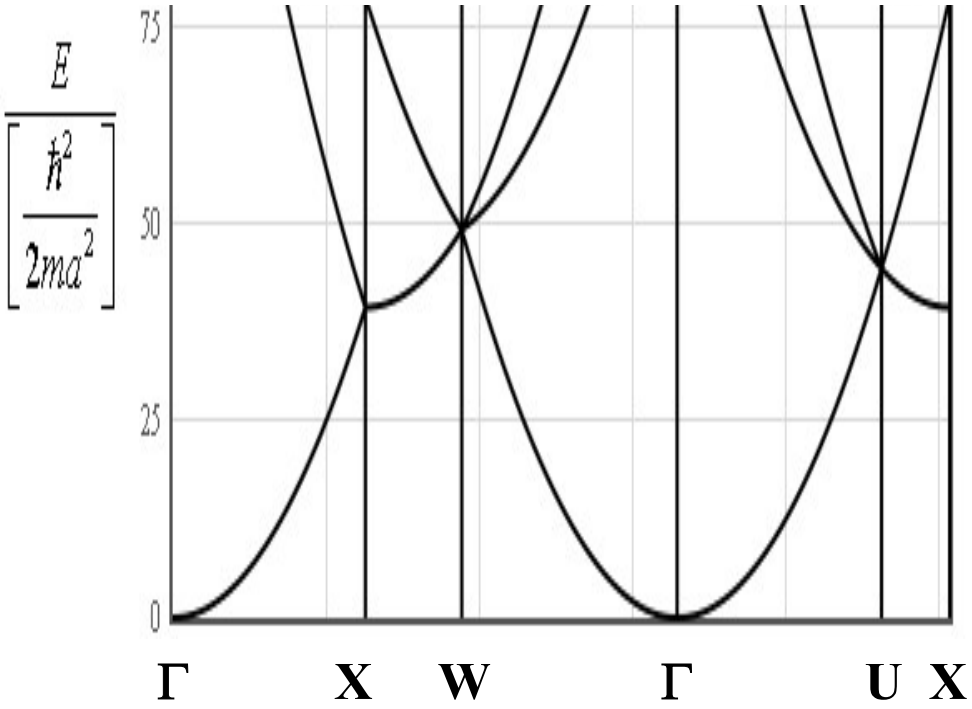
PHYSICAL REVIEW VOLUME 118, NUMBER 5 JUNE 1, 1960

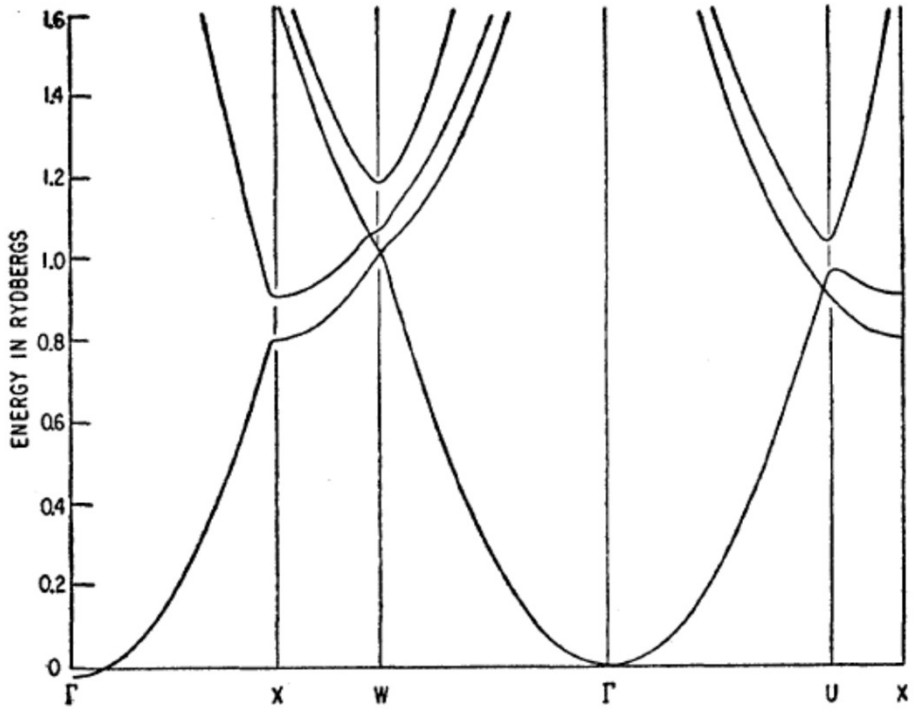
Band Structure of Aluminum

WALTER A. HARRISON
General Electric Research Laboratory, Schenectady, New York



empty lattice approximation

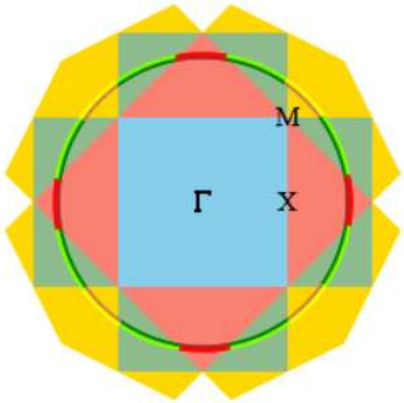




Fermi surface of a two-dimensional square lattice

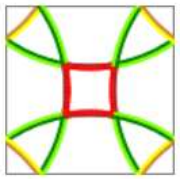
n =4.7 - + electrons/unit cell

$\frac{k_F a}{\pi}$ =1.730 $\frac{E_F}{\left[\frac{\hbar^2\pi^2}{2ma^2}\right]}$ =2.992



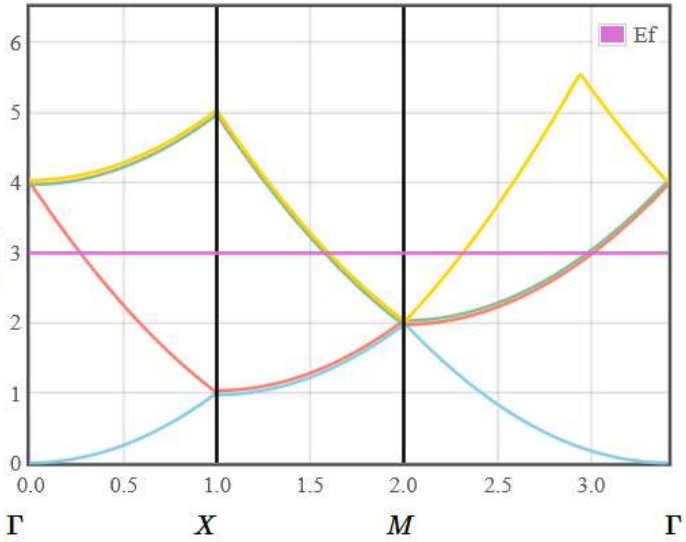
1 Bz 2 Bz 3 Bz 4 Bz

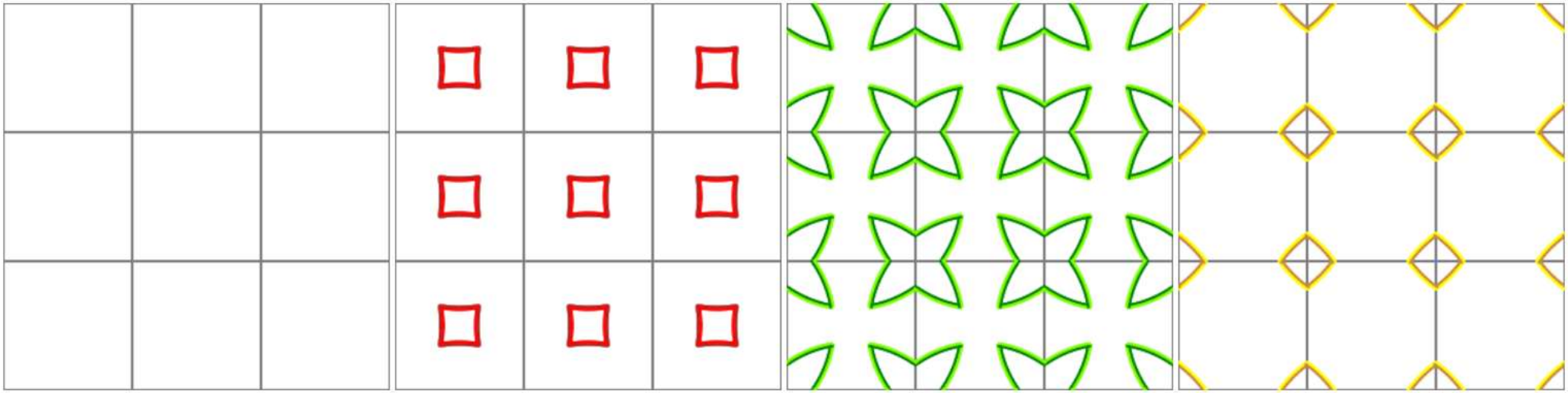
Extended Zone Scheme



Reduced Zone Scheme

$\frac{E}{\left[\frac{\hbar^2\pi^2}{2ma^2}\right]}$





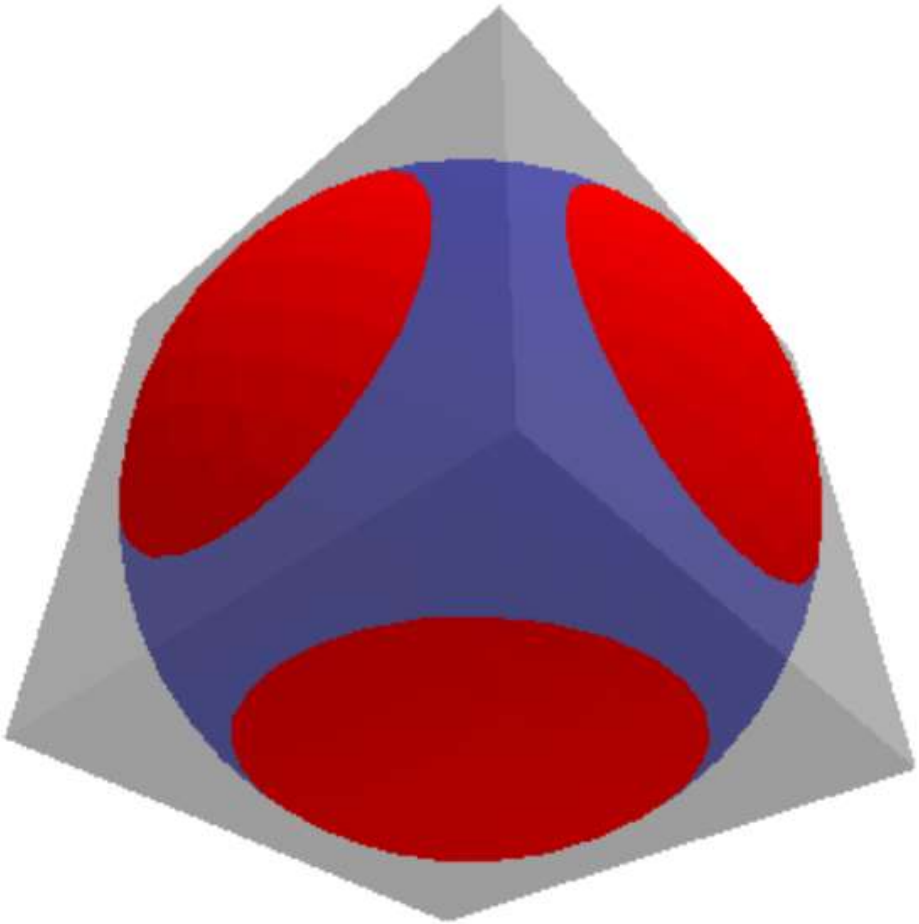
1st Brillouin Zone
Repeated Zone Scheme

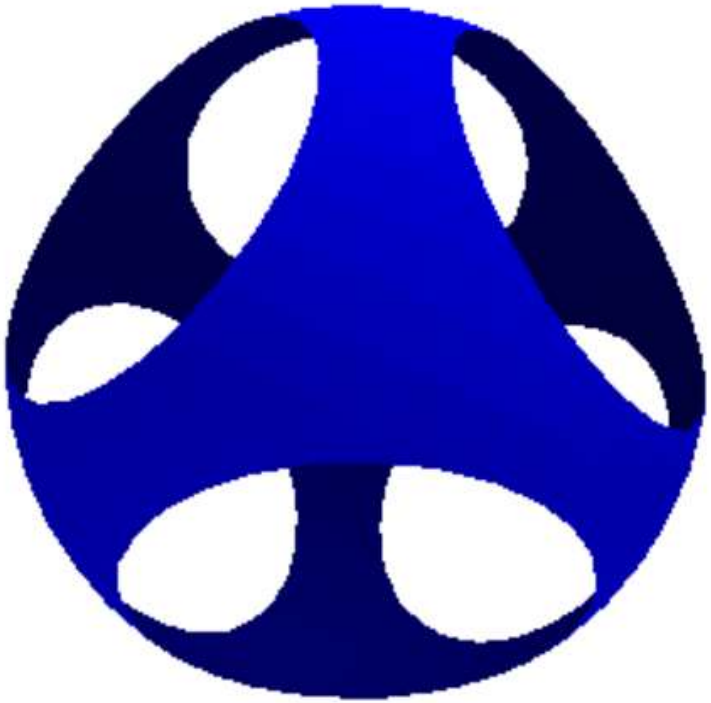
2nd Brillouin Zone
Repeated Zone Scheme

3rd Brillouin Zone
Repeated Zone Scheme

4th Brillouin Zone
Repeated Zone Scheme

Fermi Surfaces

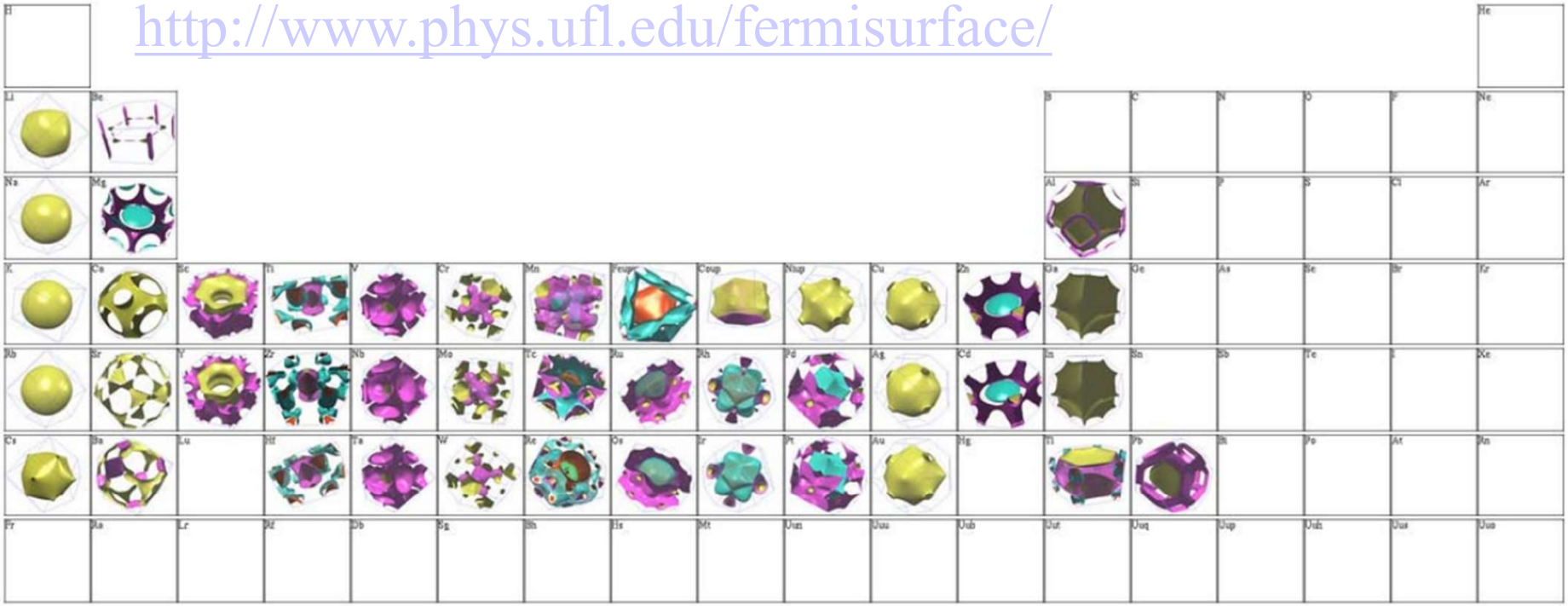




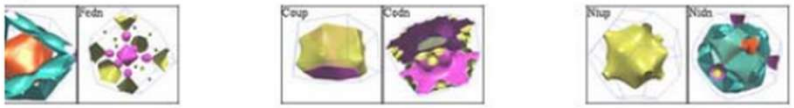
https://lampz.tugraz.at/~hadley/ss1/book/bands/3d_fermisurface/index.php

1A 2A 3B 4B 5B 6B 7B 8 1B 2B 3A 4A 5A 6A 7A NG

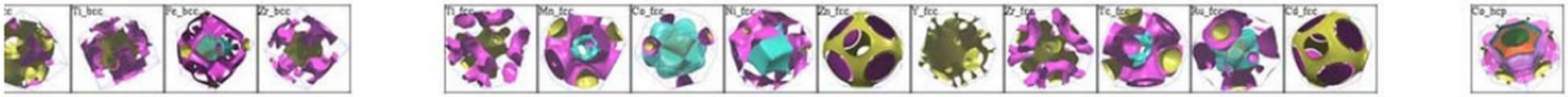
http://www.phys.ufl.edu/fermisurface/



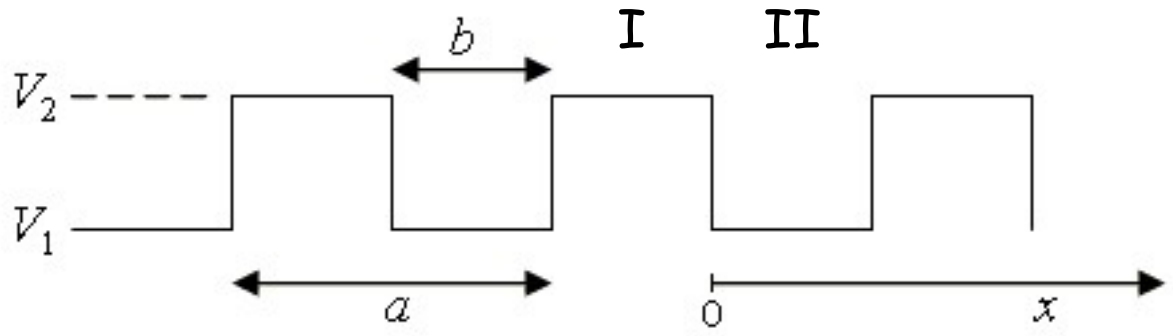
magnets :



native Structures :



A separable potential

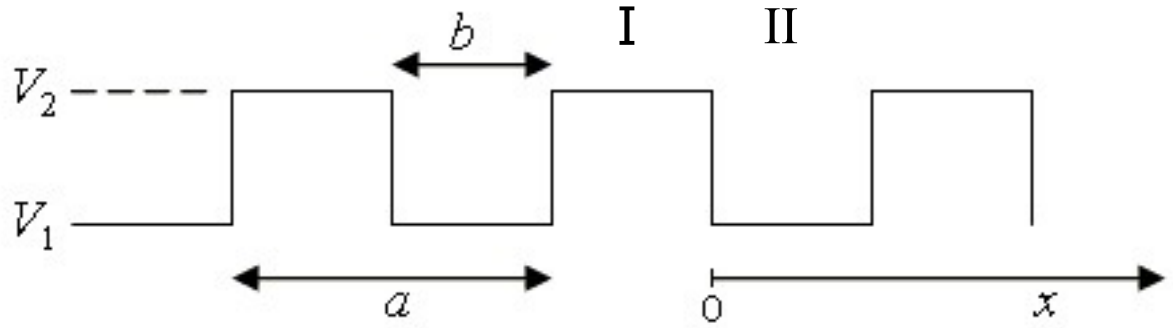


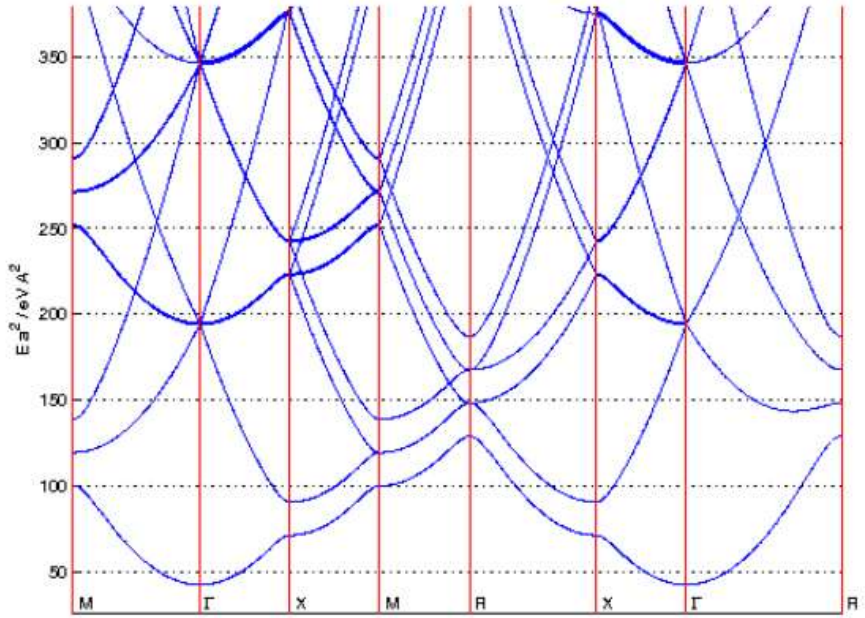
$$-\frac{\hbar^2}{2m}\nabla^2\Psi+(V(x)+V(y)+V(z))\Psi=E\Psi$$

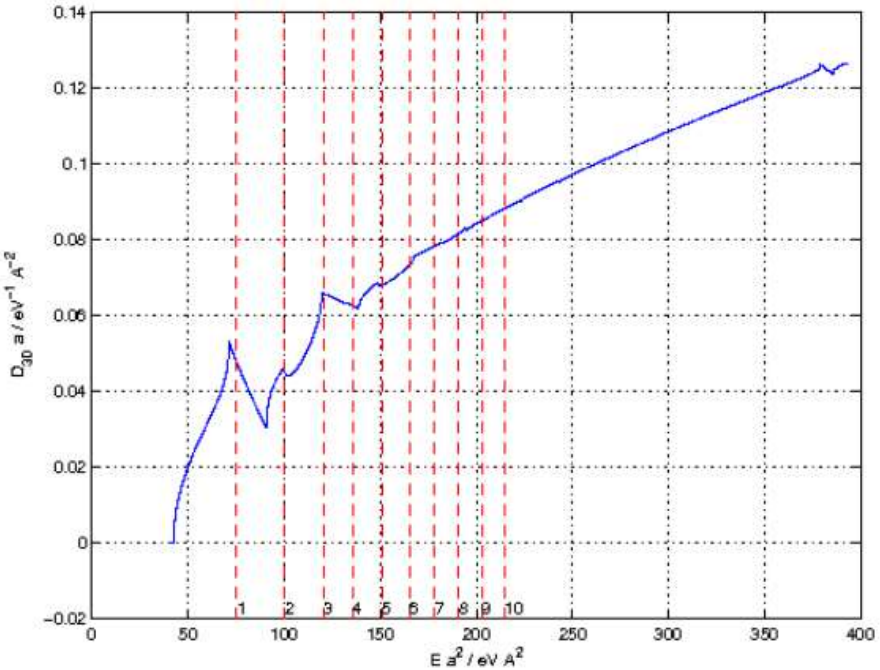
Ψ is the product of the solutions to the Kronig-Penney model.

$$\Psi(x,y,z)=\psi_{KP}(x)\psi_{KP}(y)\psi_{KP}(z)$$

A separable potential

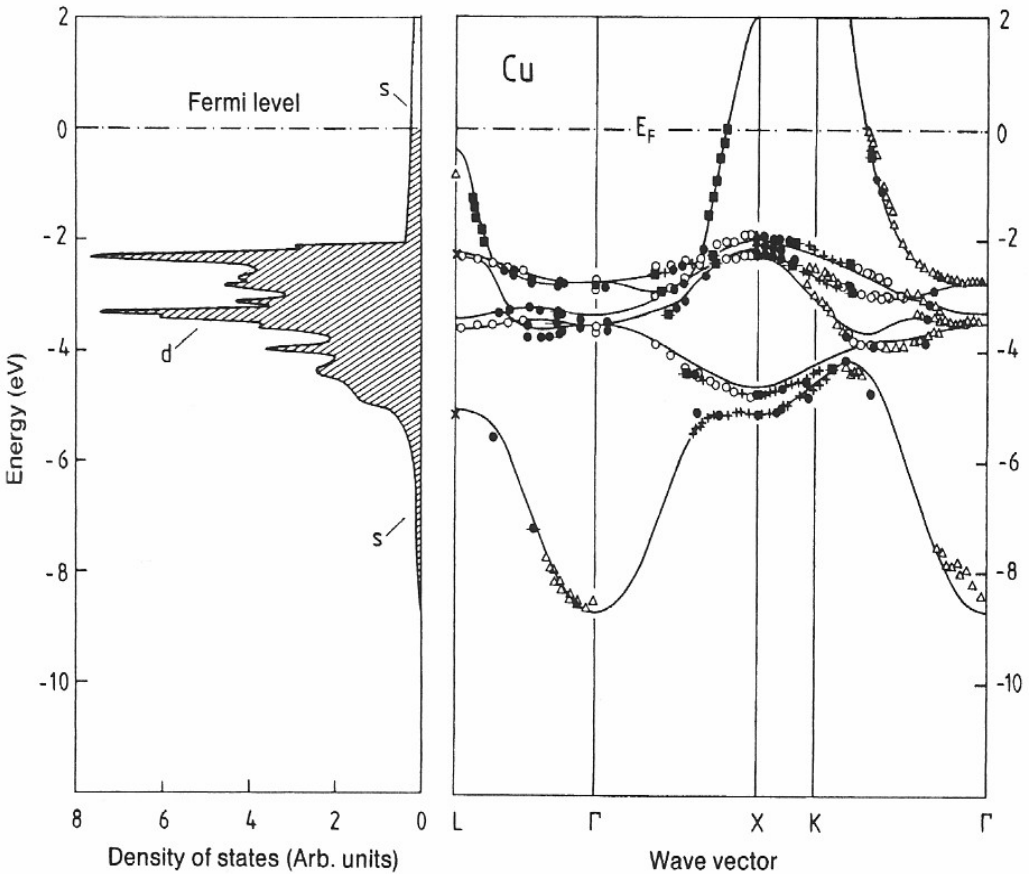


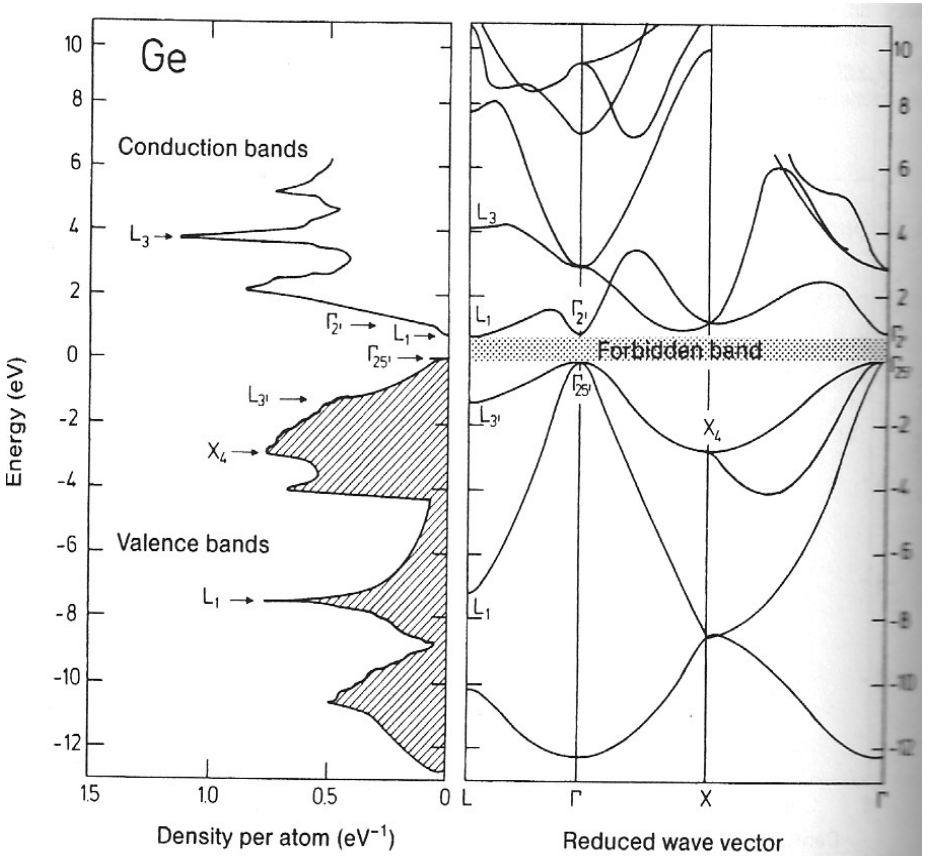




http://lampx.tugraz.at/~hadley/ss1/separablecrystals/thermo.html

Metals, semiconductors, and insulators



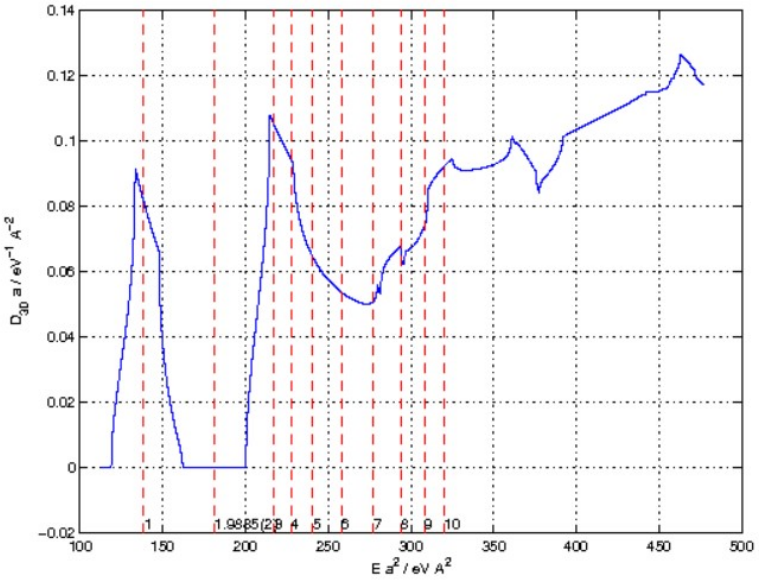


Insulators: band gap > 3 eV

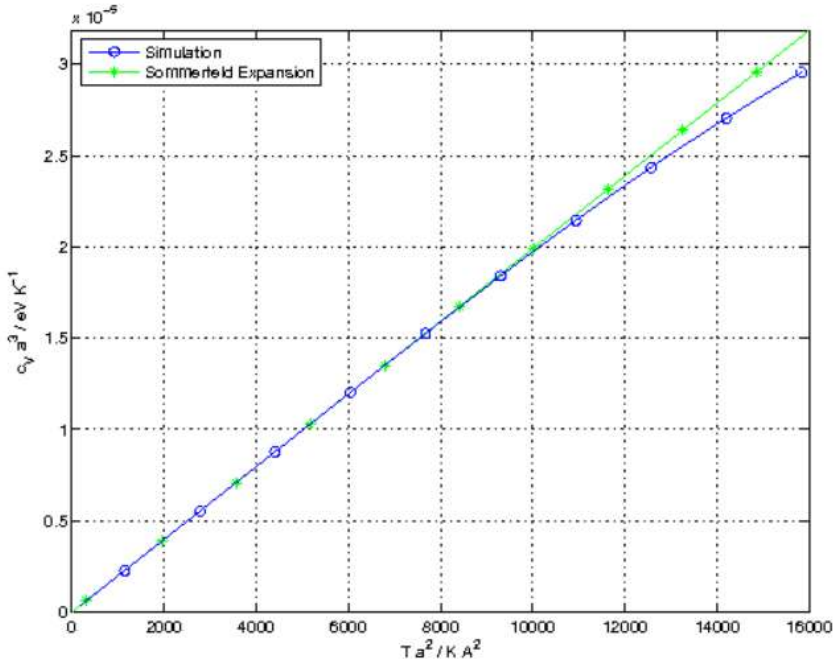
From Ibach & Lueth

The thermodynamic properties depend dramatically on the number of electrons in the primitive unit cell

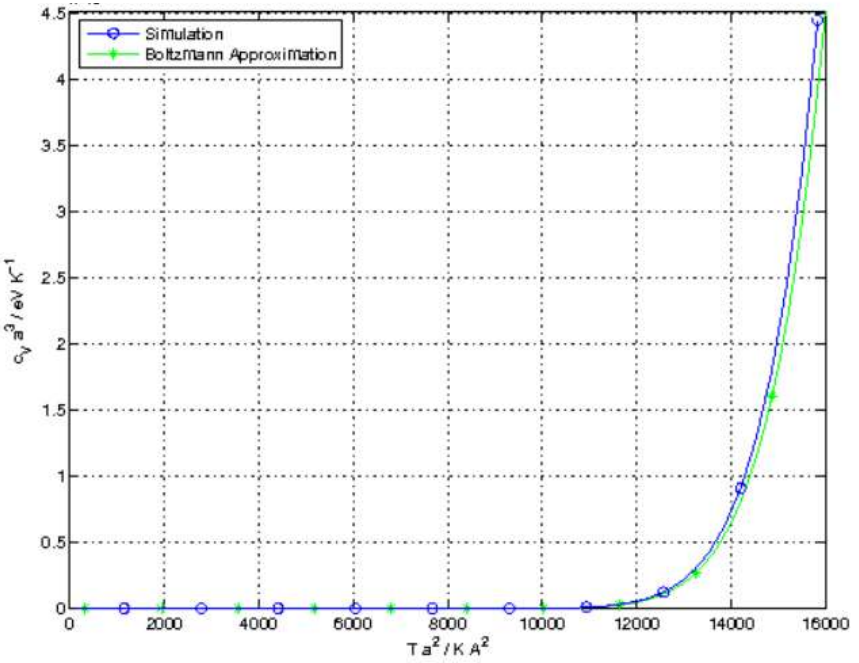
Metal
n =1



Insulator
n = 2



Specific heat c_V

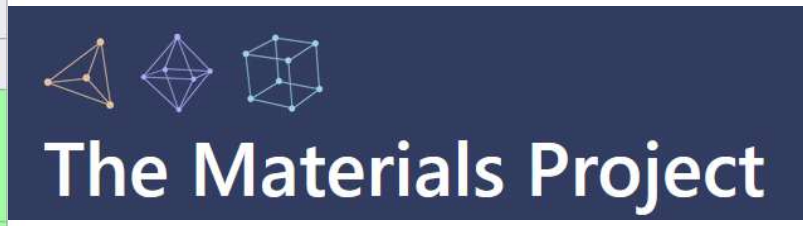


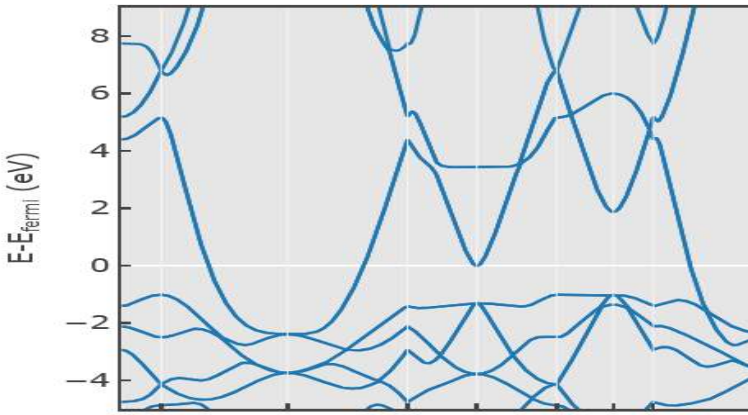
Specific heat c_V

Band structure calculations

Package	License†	Language	MPI	OpenMP	GPU	I/O libraries	Parallel I/O
ABINIT	Free, GPL	Fortran	Yes	Yes	Yes, CUDA	Yes, HDF5, NetCDF	Yes, Fortran and HDF5
ACES[1]	Free, GPL	Fortran, C++	Yes	No	Yes	Unknown	Unknown
ADF, Amsterdam Modeling Suite	Commercial	Fortran	Unknown	Unknown	Yes, CUDA	Yes, HDF5, custom	Unknown
AMPAC	Academic	Unknown	Unknown	Unknown	No	Unknown	Unknown
Atomistix ToolKit (QuantumATK)	Commercial	C++, Python	Yes	Yes	Yes, CUDA	Yes, HDF5, NetCDF	Yes, HDF5
BigDFT	Free, GPL	Fortran	Yes	Yes	Yes	Yes, HDF5, NetCDF	Yes, HDF5, NetCDF
CADPAC	Academic	Fortran	Unknown	Unknown	No	Unknown	Unknown
CASINO (QMC)	Academic	Fortran 2003	Yes	Yes	Yes, OpenACC	No	No
CASTEP	Academic, commercial	Fortran 95, Fortran 2003	Yes	Yes	No	Unknown	Unknown

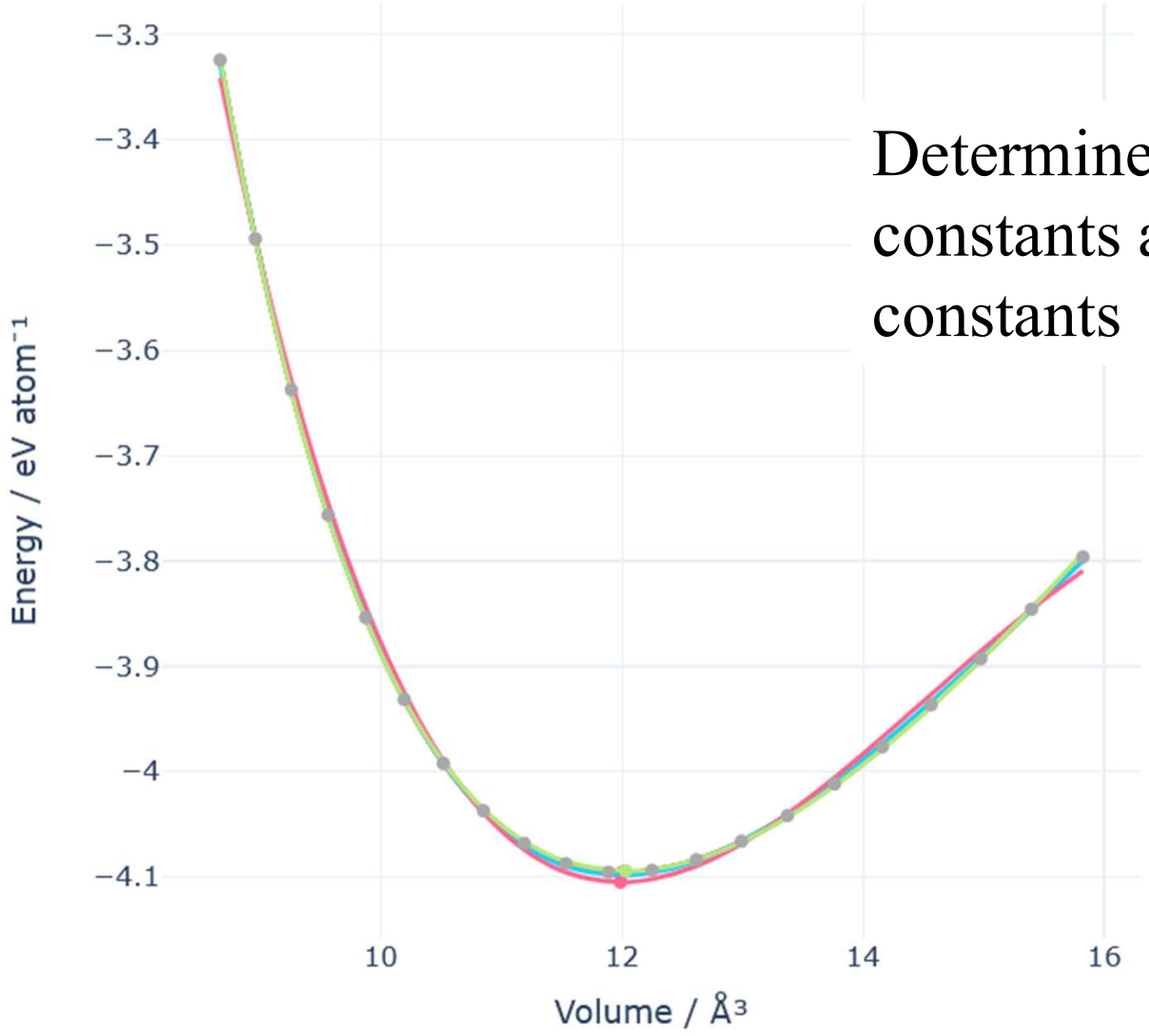
Quantum Espresso
VASP
FHI-AIMS
ABINIT





https://en.wikipedia.org/wiki/List_of_quantum_chemistry_and_solid-state_physics_software

Band structure calculations



Determine the lattice constants and spring constants