Computational Materials Physics

Center for Molecular Modeling

Department of Materials Science and Engineering

quantum numbers for a crystal

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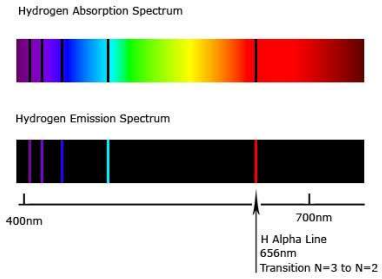
http://molmod.ugent.be
http://www.ugent.be/ea/dmse/en
my talks on Youtube: http://goo.gl/P2b1Hs

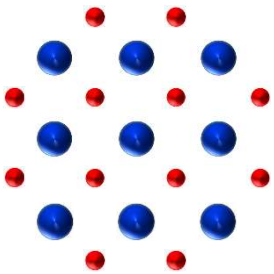
quantum numbers



Without those quantum numbers, we could not describe the experimentally observed behaviour of hydrogen atoms.

quantum numbers

solid (quantum)

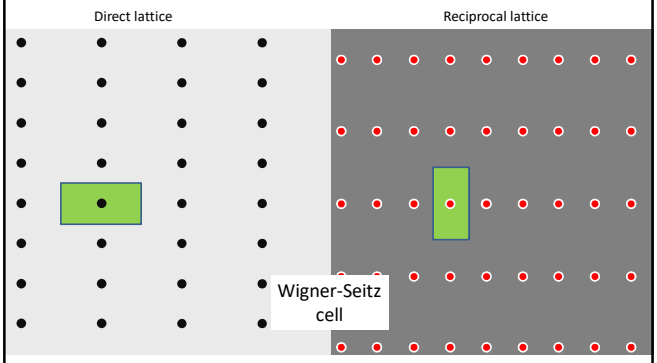


only selected energies possible.

assuming static nuclei (Born-Oppenheimer), how many degrees of freedom ?

so, how many quantum numbers do we need ?

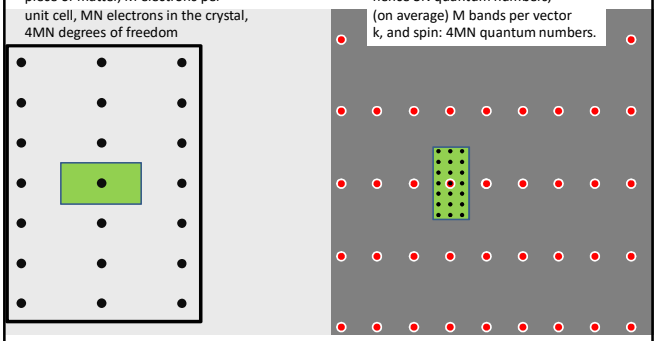
reciprocal lattice



reciprocal lattice

N unit cells in the macroscopic piece of matter, M electrons per unit cell, MN electrons in the crystal, 4MN degrees of freedom

N points in the first BZ, hence 3N quantum numbers, (on average) M bands per vector k, and spin: 4MN quantum numbers.

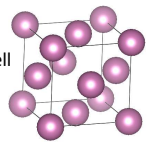


$(n, \overline{k}, s)$

overview eigenvalues:

method 1 – band structure

unit cell



overview eigenvalues:

method 1 – band structure

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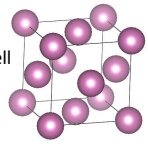
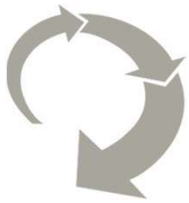
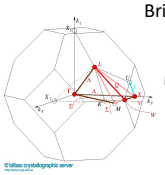




Brillouin zone (special points indicated)



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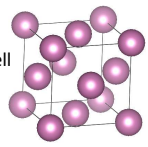

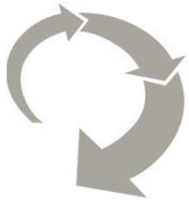

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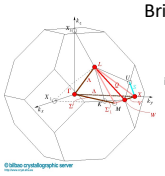
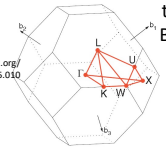


path through Brillouin zone



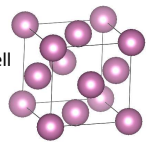
List of conventional paths in Setyawan & Curtarolo http://dx.doi.org/10.1016/j.commatsci.2010.05.010

Fig. 2. Brillouin zone of FCC lattice. Path: Γ–X–W–K–Γ–L–U–W–L–K|U–X. An example of band structure using this path is given in Fig. 27.

overview eigenvalues:

method 1 – band structure

unit cell



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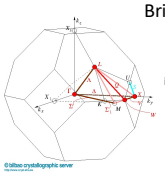

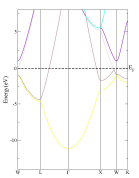

eigenvalues along path = "band structure plot" = "spaghetti plot"

path through Brillouin zone

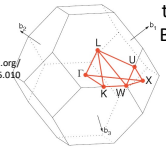

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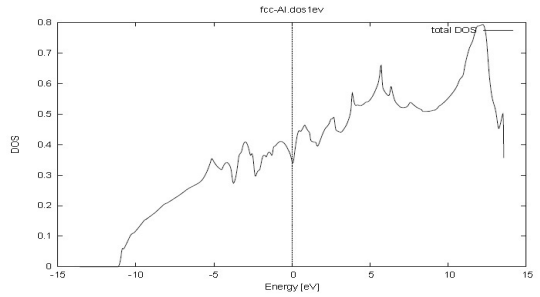
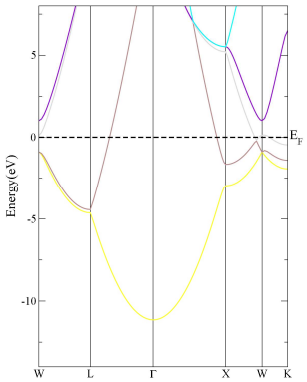
Fig. 2. Brillouin zone of FCC lattice. Path: Γ–X–W–K–Γ–L–U–W–L–K|U–X. An example of band structure using this path is given in Fig. 27.

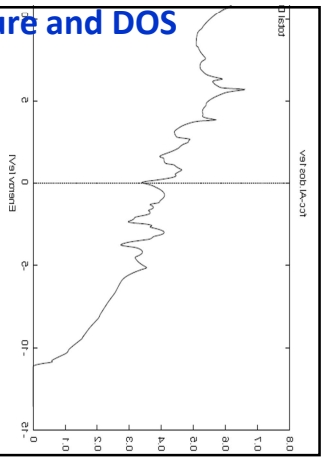
overview eigenvalues:
method 2 – DOS

For every (infinitesimally small) energy interval [E, E+dE]:
count how many k-vectors have an eigenvalue in that interval



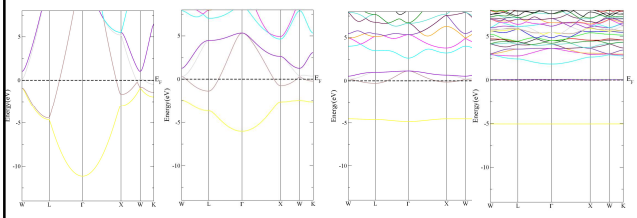
band structure and DOS





exercise: explain this

Band structure plot for ever increasing lattice parameter in fcc-Al :



a= 7.65 au a= 10.0 au a= 15.0 au a= 25.0 au

Why does the 3s band gets flat before the 3p,
and the 3p before the 4s and other unoccupied bands ?

How would a band structure plot look like for a free atom ?