First principles calculations

hand-on experiments

Ling-Ti Kong

EMail: kongIt@sjtu.edu.cn

School of Materials Science and Engineering, Shanghai Jiao Tong University

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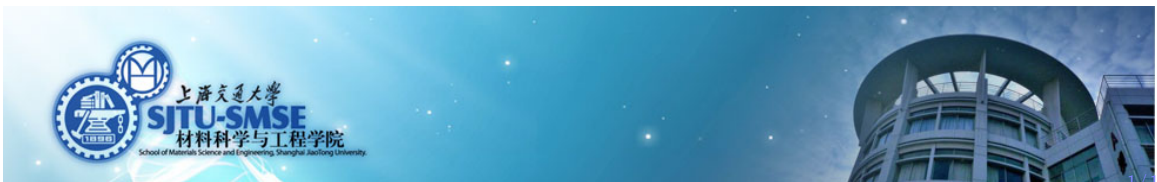


Outline

Murnaghan's Equation of states (EOS)

$$E(V) = \frac{B_0 V}{B_0'}\left[\frac{(V_0/V)^{B_0'}}{B_0'} + 1\right] - \frac{B_0 V_0}{B_0' - 1} + E_0$$

E : Total energy

E_0 : Minimum total energy

V : Volume

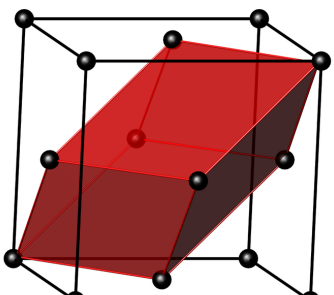
V_0 : Equilibrium volume

B_0 : Bulk modulus under equilibrium, $V \left.\frac{\partial^2 E}{\partial V^2}\right|_{V_0}$

B_0' : $\left.\frac{\partial B}{\partial P}\right|_{P_0}$

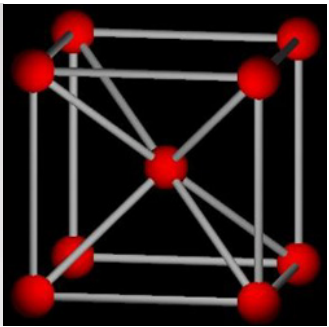
Murnaghan F D. The compressibility of media under extreme pressures. Proc. Natl. Acad. Sci. USA, 1944, 30: 244

Experimental data for fcc Cu



Lattice constant: 3.615 Å Bulk Modulus: 140 GPa

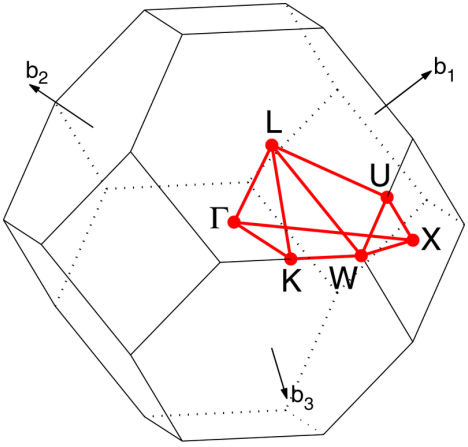
Experimental data for bcc Fe



Lattice constant: 2.8665 Å
Bulk Modulus: 170 GPa

http://www.periodictable.com/Elements/026/data.html

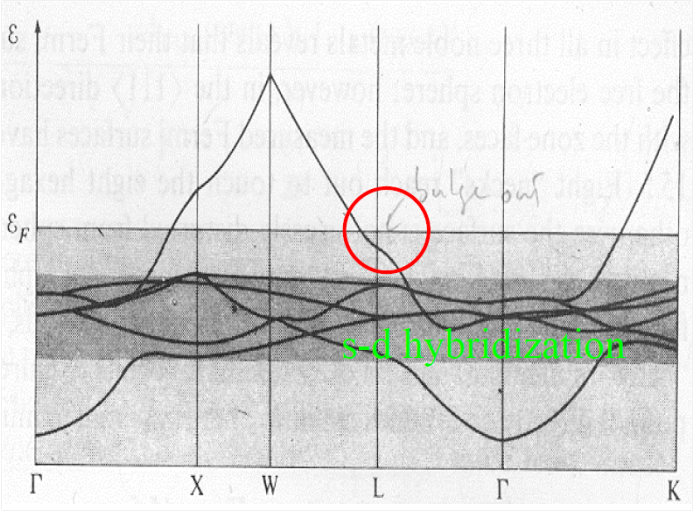
First Brillouin zone of fcc lattice



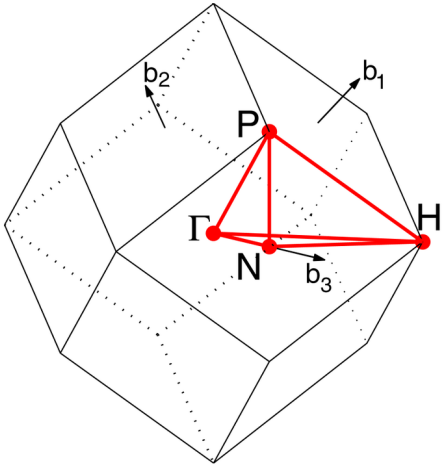
FCC path: Γ-X-W-K-Γ-L-U-W-L-K|U-X

[Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]

Band structure of fcc Cu



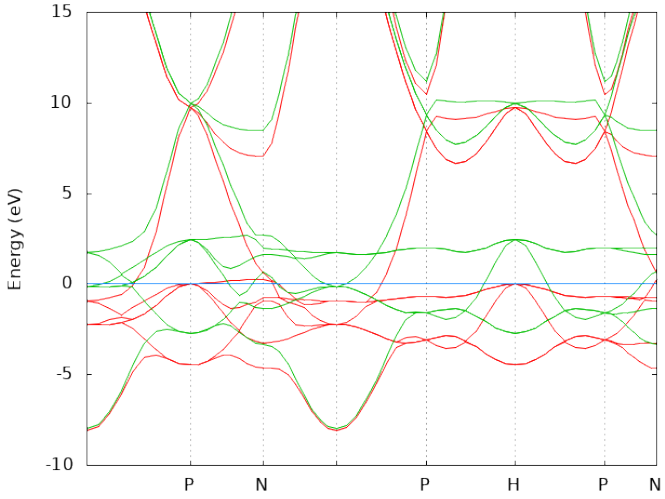
First Brillouin zone of bcc lattice



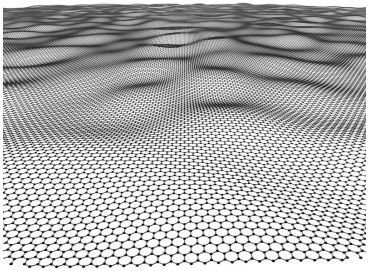
BCC path: Γ-H-N-Γ-P-H|P-N

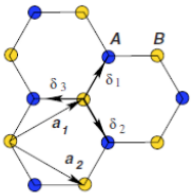
[Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]

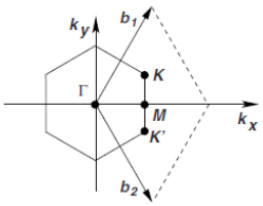
Band structure of bcc Fe



Graphene



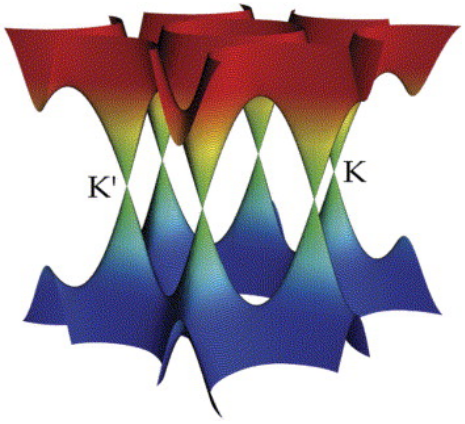


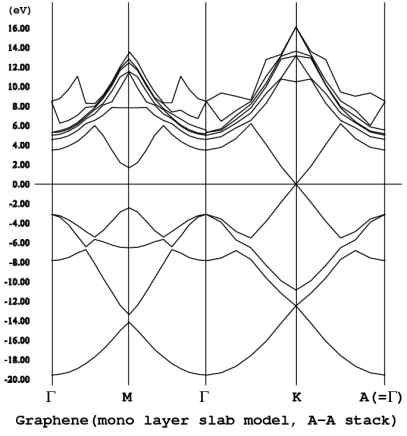


Source:
http://news.discovery.com/tech/cooling-down-electronics-with-graphene.html

http://thep-center.org/src/article_edu_e.php?article_edu_id=17

Band structure of graphene

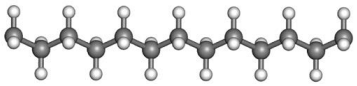


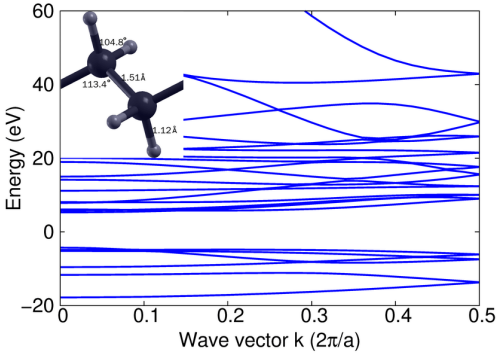


Source:
http://www.sciencedirect.com/science/article/pii/S1369702106717886

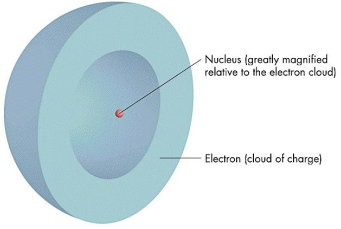
http://www.bandstructure.jp/Table/BAND/Graphene.html

Polyethylene

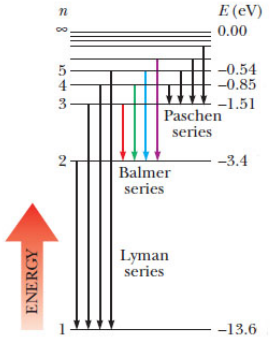




Hydrogen atom



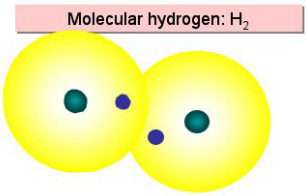
Cross section of a hydrogen atom

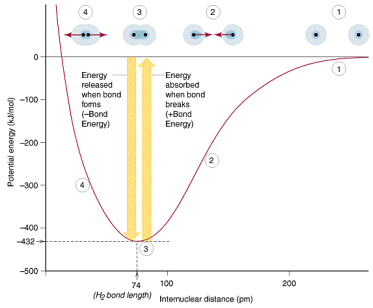


An energy level diagram for hydrogen.

$$E_n = -\frac{2\pi^2 me^4}{n^2 h^2} = -\frac{13.6\ \text{eV}}{n^2}$$

Hydrogen molecule





Bond length $b_0 = 0.74$ Å
Band energy $E_b^0 = -4.48\ \mathrm{eV} = -0.33\ \mathrm{Ry}$

Surface energy calculation

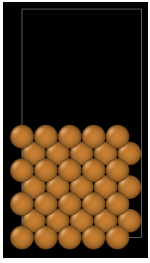
- Bulk energy calculation (reference, E_{bulk}) ;
- Static calculation for clean surface ($E_{unrelaxed}$) ;

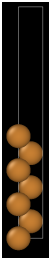
$$\gamma_{unrelaxed} = \frac{E_{unrelaxed} - N \cdot E_{bulk}}{2A}$$

- Relaxing one side of the surface while keeping the other side fixed;
- Static calculation for the relaxed structure ($E_{relaxed}$) ;

$$\gamma = \gamma_{unrelaxed} + \frac{E_{relaxed} - E_{unrelaxed}}{A}.$$

N: number of atoms in surface model. E_{bulk} in unit of eV/atom.



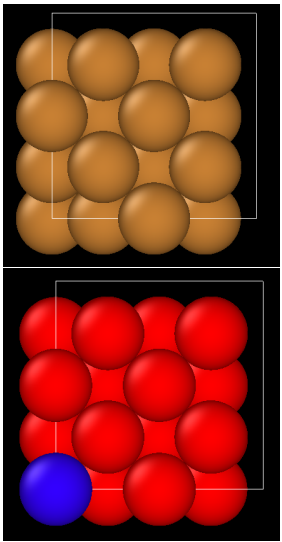


Vacancy formation energy calculation

- Bulk energy calculation (reference, E_{bulk}) ;
- Relaxation of supercell with a vacancy, and static calculation of the relaxed structure ($E_{relaxed}$) ;

$$E_v^f = E_{relaxed} - \frac{N-1}{N} E_{bulk}.$$

N: number of atoms in perfect crystal.



Homework

- Go over all the examples and finish all the remaining calculations by yourself.
- Perform DFT calculations for Al with its FCC primitive cell:
  1. Carry out convergence tests with respect to *k-mesh* size and E_{cut}.
  2. Determine the a_0 and B_0 of FCC Al by scanning a range of lattice parameters with Gaussian, Fermi-Dirac, and Methfessel-Paxton smearings, respectively.
  3. Calculate the surface energy for Al(001), Al(110), Al(111), and vacancy formation energy for Al.
  4. Compare your results to experimental data, the MD results, and DFT results in literatures.
  5. Finish an experimental report.

Due: **Dec 7th, 2022.**

http://www.periodictable.com/Elements/029/data.html