First principles calculations

hand-on experiments

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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

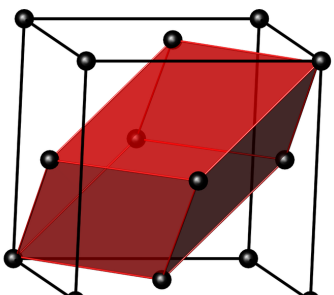
V_0 : Equilibrium volume

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

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

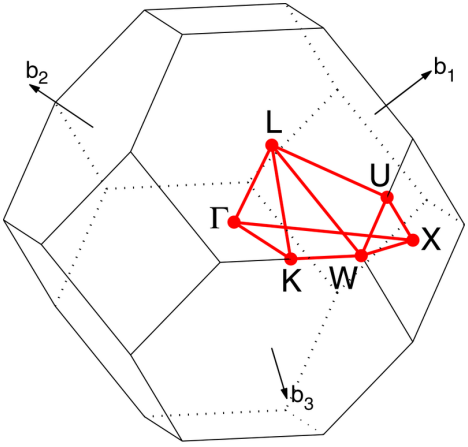
Murnaghan F D. The compressibility of media under extreme pressures. Proc. Natl. Acad. Sci. USA, 1944, 30: 244

Experimental data for fcc Cu



Lattice constant: 3.615 Å Bulk Modulus: 140 GPa

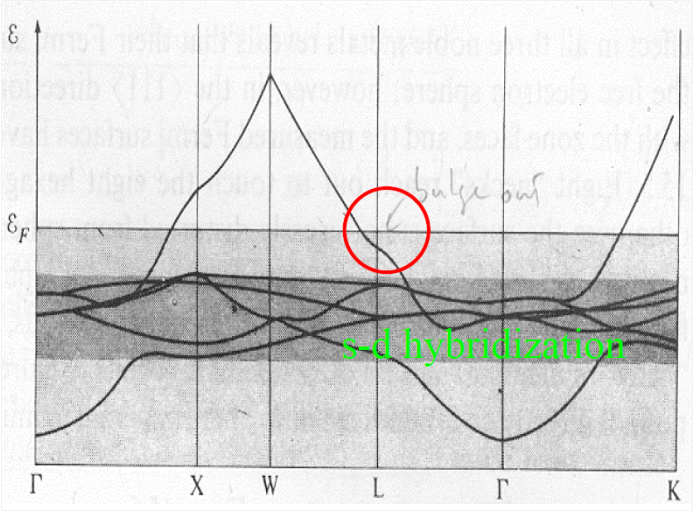
First Brillouin zone of fcc lattice



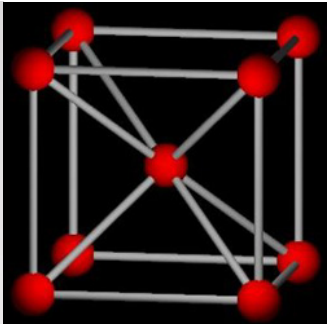
FCC path: Γ-X-W-K-Γ-L-U-W-L-K|U-X

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

Band structure of fcc Cu



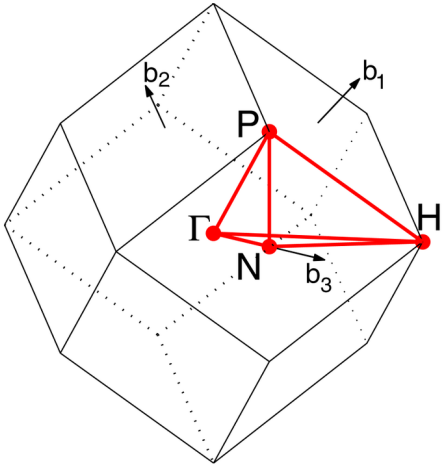
Experimental data for bcc Fe



Lattice constant: 2.8665 Å
Bulk Modulus: 170 GPa

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

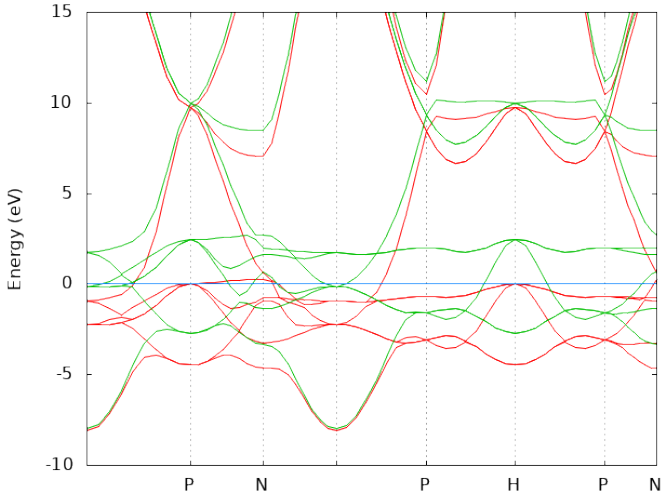
First Brillouin zone of bcc lattice



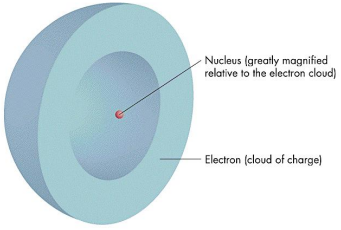
BCC path: Γ-H-N-Γ-P-H|P-N

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

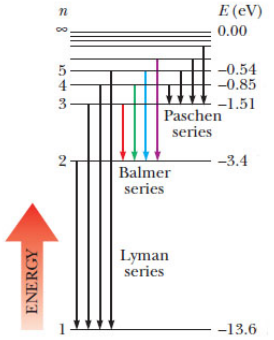
Band structure of bcc Fe



Hydrogen atom



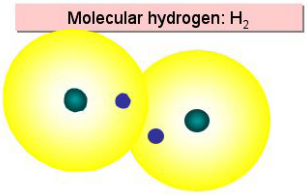
Cross section of a hydrogen atom

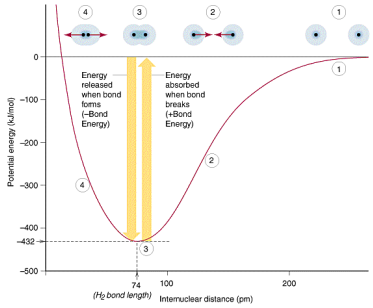


An energy level diagram for hydrogen.

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

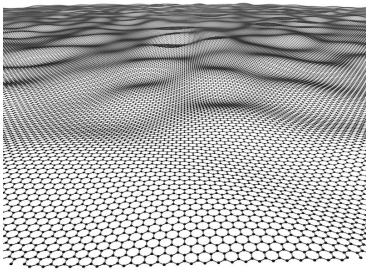
Hydrogen molecule

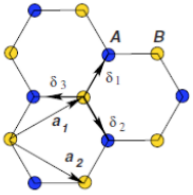


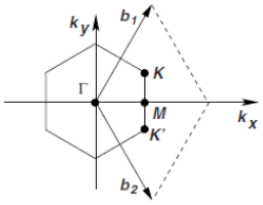


Bond length $b_0 = 0.74$ Å
Band energy $E_b^0 = -4.48\ \mathrm{eV} = -0.33\ \mathrm{Ry}$

Graphene



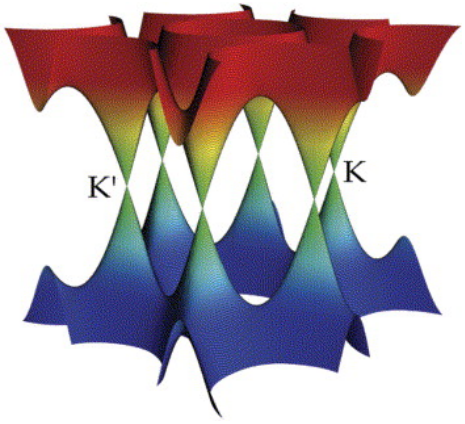


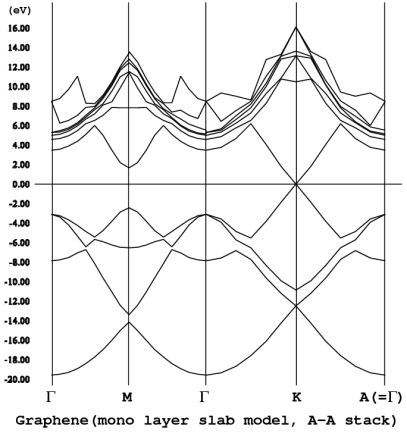


Source:
http://news.discovery.com/tech/cooling-down-electronics-with-graphene.html

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

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. Compare your a_0 and B_0 to experimental data and DFT results in literatures.
  4. Finish an experimental report.

Due: **Nov 10^{th}, 2021.**

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