Homework 1

Kyle Wodehouse

September 3, 2024

1 Syllabus Review

(a) 207 Dupont Hall

(b) 6 homework assignments

(c) 17 at very least.

(d) 'analyze and select an appropriate material for a given application' and 'select an approproate method to characterize the structure or properties of a material.'

2 Bonding Energy

a.

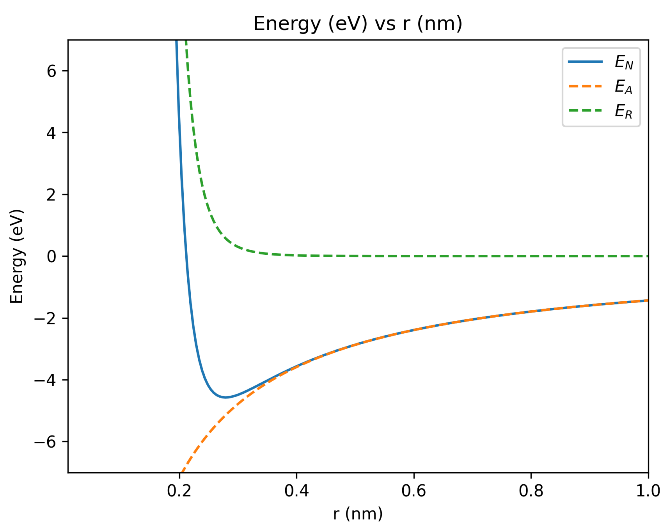


Figure 1: K^+ and Cl^- energy profile

b.

for this one I used some python code to put a vertical line at the distance where energy is minimized–*the equlibrium bond length will be when the energy is at a local minimum.* To be a little more rigorous and get some more digits I also loaded up desmos and graphically found the minimum on there as well.

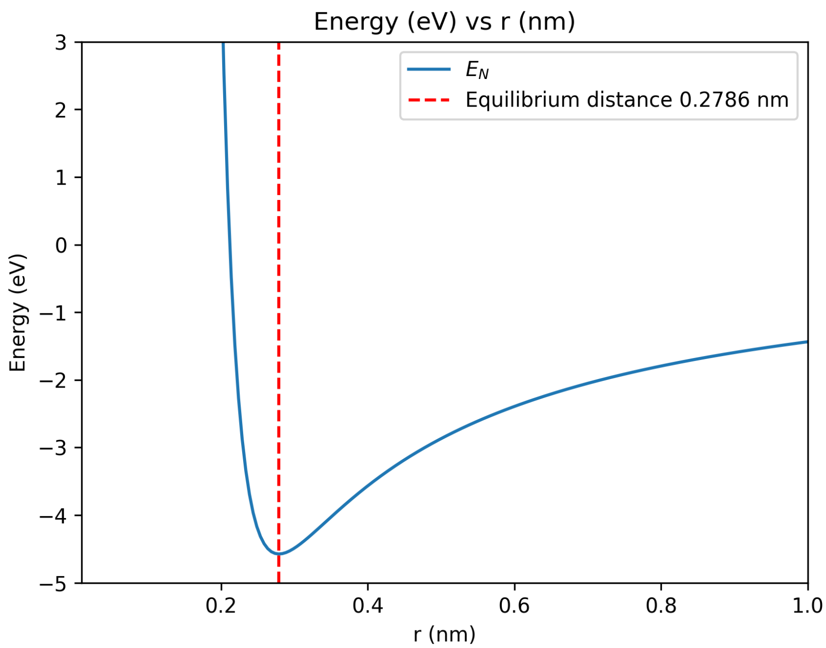


Figure 2: K^+ and Cl^- energy profile with local minimum displayed

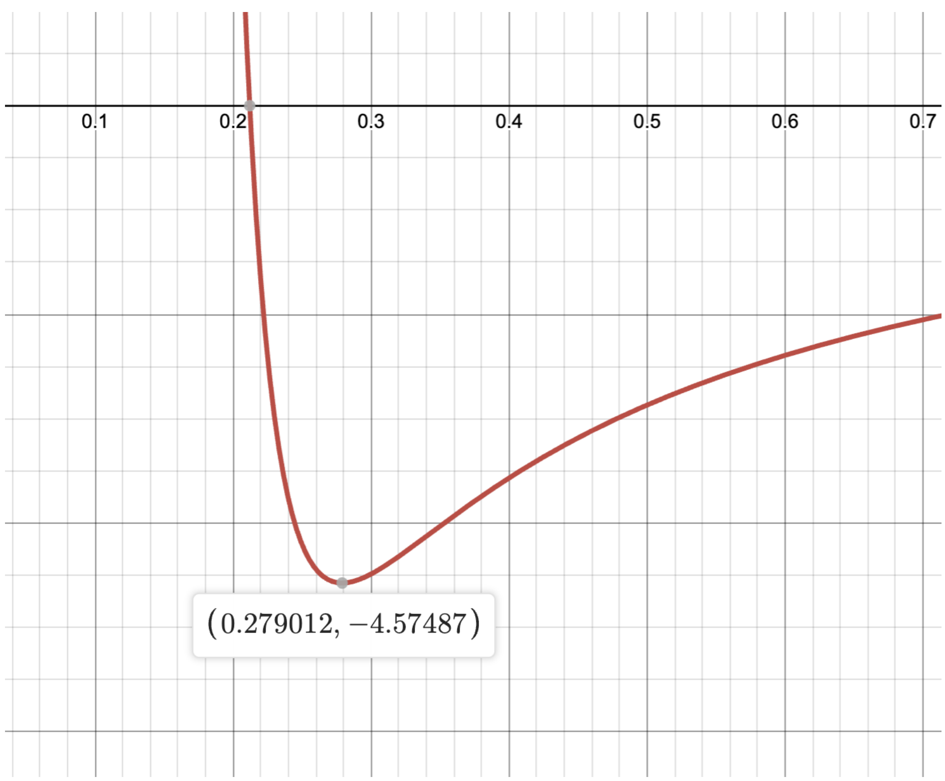


Figure 3: K^+ and Cl^- energy profile on desmos with local minimum displayed

From the desmos graph, the equlibrium spacing and the magnitude of the bonding energy are 0.279 nm and -4.57 eV respectively.

c.

To mathematically calculate it we can take the derivitive, set it equal to zero, and solve for r and then plug that into the original equation to get the energy.

At equlibrium spacing,

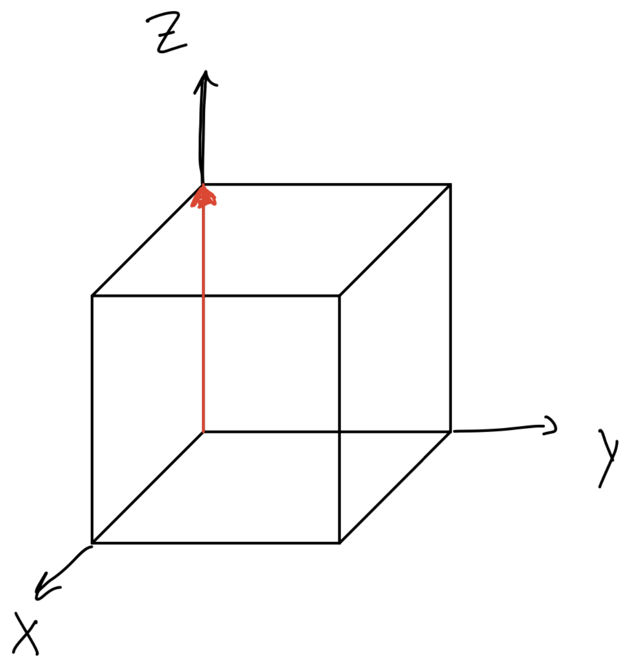
$$\begin{aligned}
\frac{dE}{dr} &= 0 \\
\frac{d}{dr}\left(-\frac{A}{r} + \frac{B}{r^9}\right) &= 0 \\
\frac{A}{r^2} - \frac{9B}{r^{10}} &= 0 \\
A &= \frac{9B}{r^8} \\
r^8 &= \frac{9B}{A} \\
r &= \left(\frac{9B}{A}\right)^{1/8} \\
&= \left(\frac{9 \times (5.86 \times 10^{-6})}{1.436}\right)^{1/8} \\
&= 0.279 \text{ nm}
\end{aligned}$$

Now we can plug this into the original equation to get the energy at the equlibrium spacing:

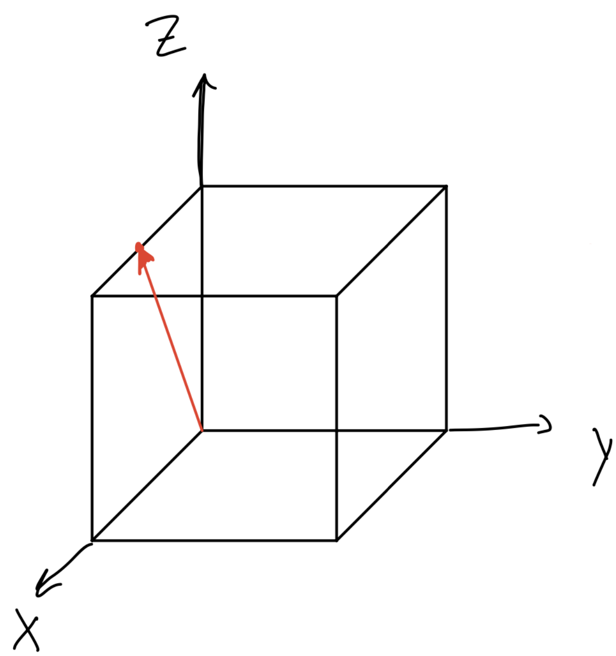
$$\begin{aligned}
E &= -\frac{1.436}{0.279} + \frac{5.86 \times 10^{-6}}{(0.279)^9} \\
&= -4.57 \text{ eV}
\end{aligned}$$

3 Miller Indices: Directions

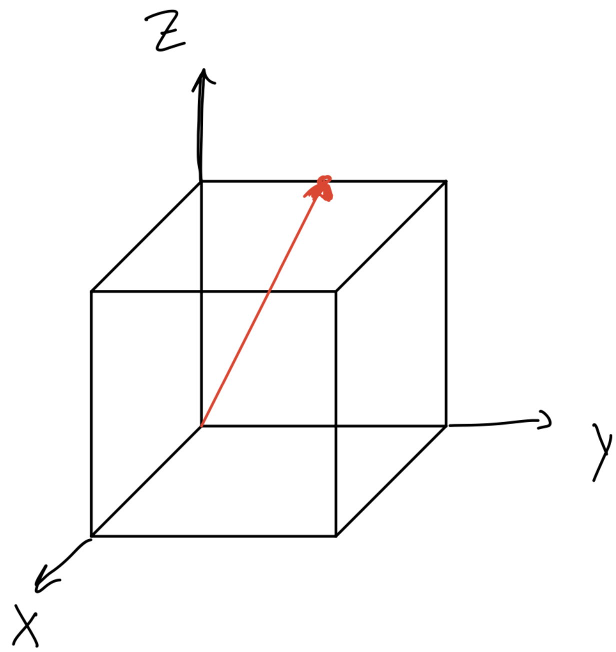
a. [001]



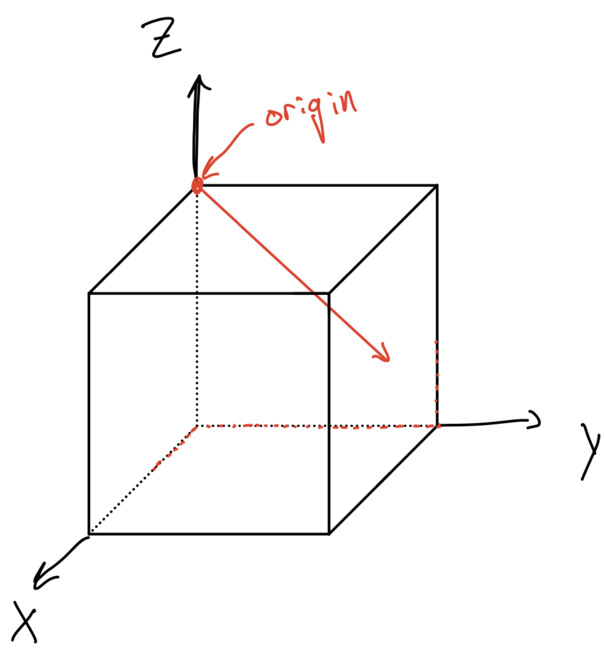
b. [102]



c. [012]

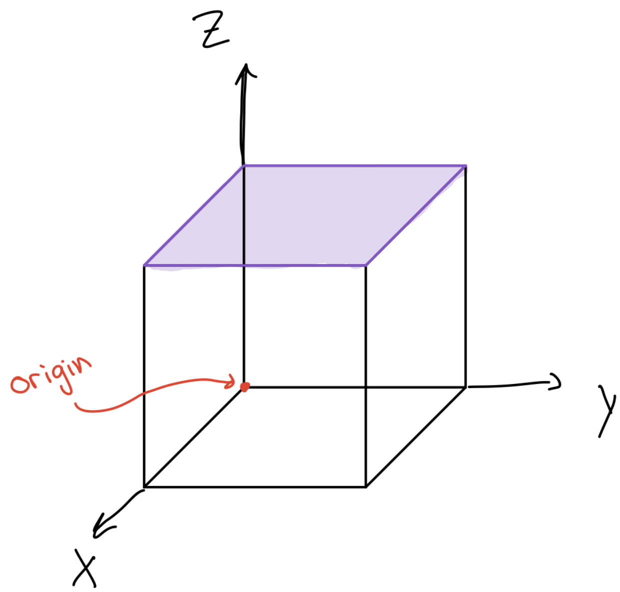


d. $[12\bar{1}]$

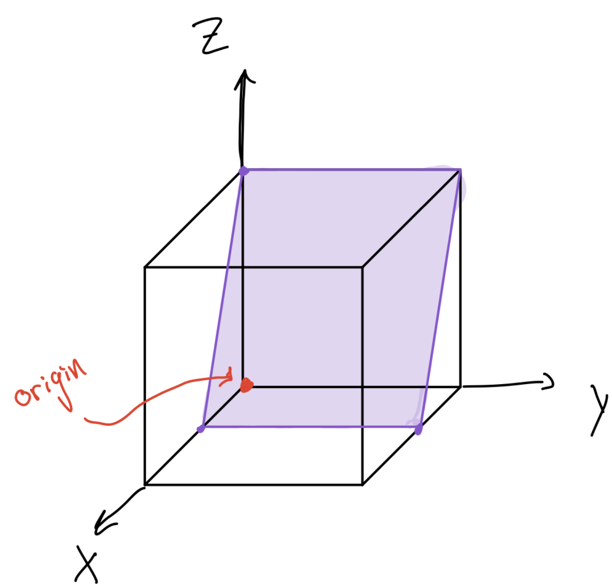


4 Miller Indices: Planes

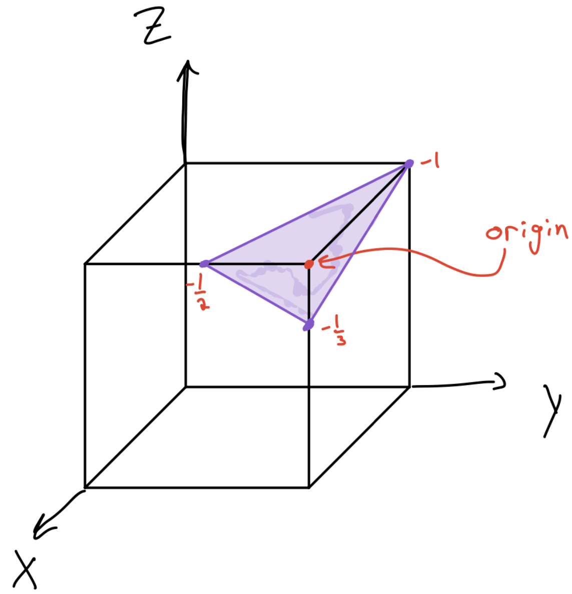
a. (001)



b. (201)



c. $(\bar{1}\bar{2}\bar{3})$



d. $(1\bar{1}\bar{2})$