Supplemental Problem for Chapter 6

1) Consider a crystal with the bcc structure that is held together by van der Waals bonds, so that the cohesion is best described by the 6-12 potential that we have used in class. (Quantitative answers can be left in terms of σ and ε)

(i) Using only nearest neighbor interactions, calculate the equilibrium spacing and the cohesive energy of this structure.

(ii) How do these quantities change when the interactions with next nearest neighbors are also included?

(ii) Qualitatively, describe how these quantities change when long range interactions with distant neighbors are included and outline the strategy that you would use to compute this effect quantitatively.

Supplemental Problem for Chapter 7

1) Write a Born-Haber cycle for TiO_2 . Provide a complete definition for all of the quantities that you use in your cycle.