Homework 1: Computational Design of Materials

Due: Oct 18, 2012

1. AlP、AlAs、AlSb and AlAs、GaAs、InAs are important compound semiconductors for optoelectronics. The first series are formed by the same cation Al, while the cation is replaced by P, As to Sb. The second series are reversed with the same anion As, but the cation is replaced by Al, Ga to In.
   Can you find out how the fundamental bandgap of the crystals (F-43M) and bond length of anion-cation vary among these species? Can you justify your first-principles simulation result with an intuitive physical picture? Does the employment of LDA or GGA for the *ab initio* calculation affect your conclusion?
   In the first series, how does the energy of cation Al change with the anion species (P, As, Sb)? In the second series, how does the energy of anion As change with the cation species (Al, Ga, In)? Can you explain your result with an intuitive physical picture?
   For the main group semiconductors C、Si、Ge、Sn, how the fundamental bandgap and bond length change with the species? Can you explain your result with an intuitive physical picture?