Assignment 1: Plot the lattice stability of hcp, fcc and liquid iron with respect to its bcc allotropic form. You may use PURE database from SGTE. – 5 marks (Due date: 17-02-2016)

Assignment 2: Plot the magnetic contribution to Gibbs energy of bcc iron as a function of temperature (300-1800 K) at 1 bar. Report enthalpy, entropy, heat capacity and Gibbs energy due to magnetic ordering of bcc iron at 400 K. What would be the most stable phase of iron at 400 K if it was not ferromagnetic? – 10 marks (Due date: 09-03-2016)

Assignment 3: Gibbs energy of AlNi phase (CsCl type) is modeled using two-sublattices as indicated below:

$$(\underline{Al},Ni)_{0.5}: (Al,\underline{Ni})_{0.5}$$

Calculate the site fractions of its sublattice constituents at 1200 K and 60 at. % of Ni. Write your program to do this. (Due date: 15-04-2016)

Given:

$$G^{AlNi}_{Al:Al} = +10083 - 4.813*T + GHSERAL$$
$$G^{AlNi}_{Ni:Ni} = +8715.08\text{-}3.556*T + GHSERNI$$
$$G^{AlNi}_{Al:Ni} = -56500 - 10.7*T + 1.4975*T*\ln(T) + 0.5*GHSERAL + 0.5*GHSERNI$$
$$G^{AlNi}_{Al:Ni} = G^{AlNi}_{Ni:Al}$$
$${}^{0}L^{AlNi}_{Al,Ni:Al} = -14225 - 5.625*T$$
$${}^{0}L^{AlNi}_{Al:Al,Ni} = {}^{0}L^{AlNi}_{Al,Ni:Al}$$
$${}^{0}L^{AlNi}_{Ni:Al,Ni} = -22050$$
$${}^{0}L^{AlNi}_{Al:Al,Ni} = {}^{0}L^{AlNi}_{Al,Ni:Ni}$$
$${}^{1}L^{AlNi}_{Ni:Al,Ni} = +1115$$
$${}^{1}L^{AlNi}_{Al,Ni:Ni} = {}^{1}L^{AlNi}_{Ni:Al,Ni}$$
$$GHSERAL = -11278.4 + 188.684*T - 31.7482*T*\ln(T) - 1.231e{+}028*T**(-9)$$
$$GHSERNI = -5179.16 + 117.854*T - 22.096*T*\ln(T) - 0.0048407*T**2$$

Assignment 4: Given the following data on $\Delta_{mix}H_m$ (J. mol^{-1}) corresponding to the limiting binary systems of Ni-Ti-V-Zr, plot $\Delta_{mix}H_m$ for $Nb_{10}Ti_{30}V_{60-y}Zr_y$ from y=0 to 60 at.% Zr using Muggianu, Colinet, and Kohler extrapolation methods (single plot with three curves, clearly marking each curve). Also report the numerical values of $\Delta_{mix}H_m$ for an equiatomic quaternary alloy. (Due date: 22-04-2016)

System	$\Delta_{mix}H_m$
Nb-Ti	$x_{Nb}x_{Ti}(+3000)$
Nb-V	$x_{Nb}x_{V}(-1875)$
Nb-Zr	$x_{Nb}x_{Zr}(-10311+6709(x_{Nb}-x_{Zr}))$
Ti-V	$x_{Ti}x_{V}(+7600+2200(x_{Ti}-x_{V}))$
Ti-Zr	$x_{Ti}x_{Zr}(-968)$
V-Zr	$x_{V}x_{Zr}(-14900+3000x_{Zr}+1000\,x_{Zr}^2)$

Assignment 5: Using Thermo-Calc compute how the equilibrium partial pressures of the most dominant gas specie of a gas mixture, initially consisting of equimolar amounts of SO_3 and O_2, vary as a function of temperature from 300 to 1500 K at 2 bar. You may use PSUB database. (Due date: 26-04-2016)