Assignments: MM6010 — **Computational Materials Thermodynamics**

<u>Assignment 1</u>: 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)