Advanced Materials Modeling
Homework 4

***Notes**: In multiple choice problems explain your answer. Add references if needed. Upload solution as a single file "YourName.pdf" or "YourName.zip".*

1. Which thermodynamic potential is minimized in thermodynamic equilibrium:

(A) at constant temperature and volume

(B) at constant temperature and pressure

2. A system consists of three non-interacting parts A, B, C. Subsystem A can be in one of W_1 microstates, subsystem B - W_2 microstates, subsystem C - W_3 microstates. Write the formula for the entropy of the whole system

3. What is the value of chemical potential of N_2 molecule (in eV) at 500 K and pressure 100 kPa? Determine the value with respect to the reference chemical potential at T = 0 K. Explain your answer in detail.
Hint:
Use data from thermochemical tables: https://janaf.nist.gov/

4. What is the value of the chemical potential of an atom A in thermodynamic equilibrium between all phases containing A, if the chemical potential of A_3 molecule in the gas phase is equal μ? Explain your answer

5. Derive the formula for the dependence of defect concentration on temerature. The free energy of defect formation at very small concentrations is ΔG_f. The defects interact with each other according to the formula $V(n) = V_0(n \ln n - n)$, where $n = N/N_0$ is the relative concentration of defects with respect to the concentration of possible defect sites, $V(n)$ is the interaction energy per unit volume, and V_0 is a constant. Dependence of the defect interaction energy on their distribution can be neglected. Assume that the concentration of defects is much smaller than the concentration of possible defect sites. For which values of V_0 this assumption is valid?