Physical Chemistry of Materials 1 **Exam I_** 2021/4/17

a. Closed-book exam, no note, and no calculator.
b. Total 5 questions, and each question is worth 10 points.
c. For brief answers in any question, please explain within several sentences, and with schematic figures if necessary.
d. Any cheating = F grade.

1. (a) By considering an ideal monatomic gas, and possible number of microstates of one atom or N atoms being in a given volume, please derive the relation of entropy change when an ideal gas expands isothermally from V_i to V_f. Your derivation by this logic does not need the 2nd law of thermodynamics. (b) By using the first and second laws of thermodynamics, please explain and derive the criteria for non-equilibrium (irreversible) system at constant temperature and pressure.

2. After measuring the heat capacity of a material experimentally, we can calculate the Gibbs free energy as a function of temperature. Please explain and derive how you can determine the Gibbs free energy of this material from the measured heat capacity.

3. (a) Assuming that the entropy S and the statistical number Ω of a physical system are related through an arbitrary functional form $S = f(\Omega)$, please show that the additive character of S and the multiplicative character of Ω necessarily require the function $f(\Omega)$ to be of the form $S \propto \ln \Omega$. (b) Please explain the meaning of proportionality k_B for this entropy relation.

4. Consider two physical systems, 1 and 2, which are separately in equilibrium. By considering two possible microstates Ω_1 (N_1, V_1, U_1) and Ω_2 (N_2, V_2, U_2), and allowing an exchange of energy U with fixed (N_1, V_1) and (N_2, V_2) in equilibrium in contact, please derive that $\partial \ln \Omega_1 / \partial U_1 = \partial \ln \Omega_2 / \partial U_2$. This clarifies the 2nd law of thermodynamics in a reversible system.

5. (a) For the first-order and second-order phase transitions for a pure (single-component) material, please plot the following functions as a function of temperature through the transition temperature: Gibbs free energy, chemical potential, heat capacity, enthalpy, volume, and entropy. Please plot these six schematic values from 0 K to above the transition temperature. (b) Can we have a second-order phase transition in a solid-liquid transition? Why or why not?