

97 年第一學期

開課系所: 化學研究所

課程名稱: 高等物理化學(專論)一

課程編號: 223 M1310/223 D1310

授課老師: 牟中原教授 (Email: cymou@ntu.edu.tw)

上課時間: 每週二第 5,6 節,週四第 2 節

上課地點: 待訂

面談:台大凝態中心暨物理系館 1022 室

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教科書: Chemical Thermodynamics of Materials: Macroscopic and  
microscopic aspects, John Wiley

Author: Stolen Grande

This course is designed to teach chemical thermodynamics with a strong connecting with modern materials chemistry and physics. The course on chemical thermodynamics should change its orientation from ideal gas and ideal solution to more emphasis on solid state of materials. Thus subjects such as phase diagram and surfaces would be emphasized instead. I intend to follow the above textbook mostly. However, near the end of semester, I will study a few recent research papers.

## 1 Thermodynamic foundations

### 1.1 Basic concepts

### 1.2 The first law of thermodynamics

### 1.3 The second and third laws of thermodynamics

### 1.4 Open systems

## 2 Single-component systems

### 2.1 Phases, phase transitions and phase diagrams

### 2.2 The gas phase

### 2.3 Condensed phases

## 3 Solution thermodynamics

### 3.1 Fundamental definitions

### 3.2 Thermodynamics of solutions

### 3.3 Standard states

### 3.4 Analytical solution models

### 3.5 Integration of the Gibbs–Duhem equation

## 4 Phase diagrams

### 4.1 Binary phase diagrams from thermodynamics

4.2 Multi-component systems

4.3 Predominance diagrams

5 Phase stability

5.1 Supercooling of liquids – superheating of crystals

5.2 Fluctuations and instability

5.3 Metastable phase equilibria and kinetics

6 Surfaces, interfaces and adsorption

6.1 Thermodynamics of interfaces

6.2 Surface effects on heterogeneous phase equilibria

6.3 Adsorption and segregation

7 Trends in enthalpy of formation

7.1 Compound energetics: trends

7.2 Compound energetics: rationalization schemes

7.3 Solution energetics: trends and rationalization schemes

8. Molecular Partition function

8.1 Canonical Ensemble

8.2 Translational partition function

8.3 Rotational Partition function

8.4 Vibrational partition function

8.5 Absolute entropy

9 Heat capacity and entropy

9.1 Simple models for molecules and crystals

9.2 Lattice heat capacity

9.3 Vibrational entropy

9.4 Heat capacity contributions of electronic origin

9.5 Heat capacity of disordered systems

10 Atomistic solution models

10.1 Lattice models for solutions

10.2 Solutions with more than one sub-lattice

10.3 Order–disorder

10.4 Non-stoichiometric compounds

成績計算： 期中考 期末考