Cem 484: Molecular Thermodynamics

- Prof. Liddick
- Office: NSCL 1006
- Email: liddick@chemistry.msu.edu
- Office hours:
  - Tues. 8 – 9:30 am
  - Wed. 1:30 – 3:00 pm

TAs and office hour

- TAs
  - Jared Hansen
  - Zhongqi Jin
- Recitations
  - Sec 1, Rm. 110 – Thurs. 10:20 am – 11:10 am, JH
  - Sec 2, Rm. 109 – Wed. 9:10 am 10:00 am, JH
  - Sec 3, Rm. 109 – Fri. 11:30 am – 12:20 pm, ZJ
  - Sec 4, Rm. 109 – Fri. 9:10 am – 10:00 am, ZJ

Grading scale

- Final grade based on average of in-class exams
- Exams – 4 in-class exams
  - All exams are cumulative
  - Extra credit questions on each exam
- Iclicker – treated as extra credit and added to final score
- Attendance (class and recitation) is not mandatory – but can help

Avg.	Grade
>85	4.0
80 – 84.9	3.5
75 – 79.9	3.0
65 – 74.9	2.5
60 – 64.9	2.0
55 – 59.9	1.5
50 – 54.9	1.0
<50	0.0

Syllabus

- Webpage - http://www2.chemistry.msu.edu/courses/cem484/index.html
- Three main topics in cem 484
  - Molecular spectroscopy
  - Statistical Thermodynamics
  - Thermodynamics
- Link between the concepts from introductory chemistry (macroscopic) and studies from cem 483 (microscopic)

Connections – simple gas molecules

Microscopic

- Quantum mechanics
- Molecular Orbital diagrams
- H_2

Macroscopic

- Chemical Thermodynamics
- Gases characterized by P,V,T
- Heat capacities

- Want to know how to go between these two regimes
- Basis of modern chemistry

Connections – simple gas molecules

Microscopic

- H_2 atom
- What is the structure, nature of bonding and energy states?
- Verified with measurements – molecular spectroscopy

Macroscopic

- Chemical Thermodynamics
- Is a chemical reaction allowed?
- Where is the equilibrium?
- Does it release heat?
- How can it be manipulated?

Connections

Quantum Mechanics

- State of system is completely defined by its wavefunction,
- Physical observables replaced by operators
- Can only measure eigenvalues of operator
- Average value of an observable corresponds to operator
- Wavefunction of system can evolve in time

Thermodynamics

- Two bodies in thermal equilibrium are at the same temperature
- Conservation of energy
- No real process is reversible
- Entropy of a pure perfect substance at 0 K = 0.

Connections – simple gas molecules

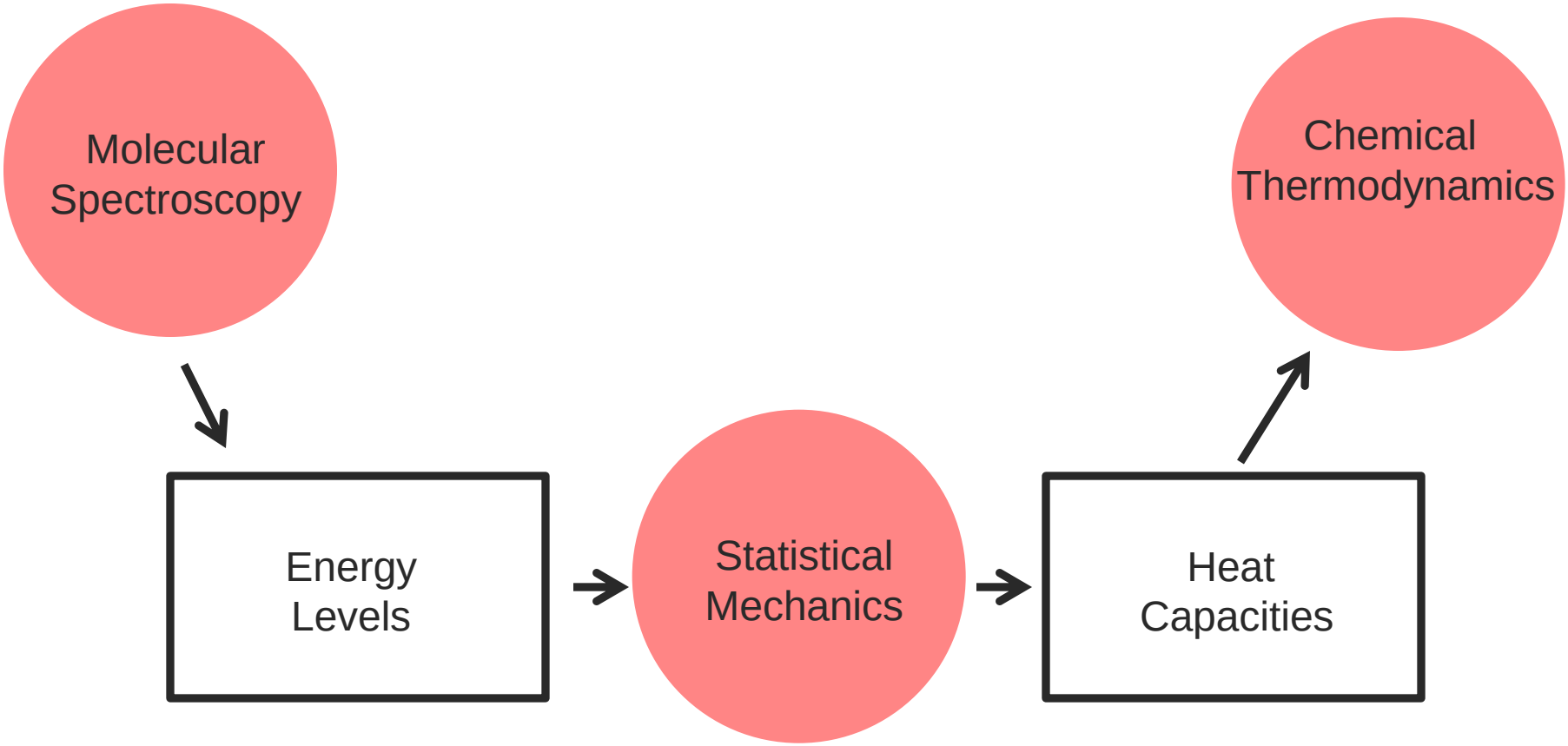
Microscopic

- $H_{elec} + H_{vib} + H_{rot}$
- UV/Vis spectroscopy
- IR spectroscopy
- Microwave spectroscopy

Macroscopic

- Chemical predictions from thermodynamic state functions
  - ΔU_{sys} – internal energy
  - ΔH_{sys} – enthalpy
  - ΔS_{sys} – entropy
  - ΔA_{sys} – helmoltz free energy
  - ΔG_{sys} – gibbs free energy
- Measure / assign some and use reaction to predict remainder

Overview


Molecular Spectroscopy
Chemical Thermodynamics
Energy Levels
Statistical Mechanics
Heat Capacities