



"From microscopic to macroscopic  
using classical physics and  
molecular modelling"

Using research tools for undergraduate teaching

Simon Halstead



# My Background

- ▶ I am a (Physical) Chemist
- ▶ Based in China
- ▶ Involved in teaching for the past 10 years
  - ▶ PhD
  - ▶ Kindergarten



# Chemistry

- ▶ Full of *qualitative* reasoning
  - ▶ Mechanisms
  - ▶ Structure – property relationships
  - ▶ Chemical intuition
- ▶ Chemists (undergraduates) dislike maths
- ▶ Thinking like a physicist:

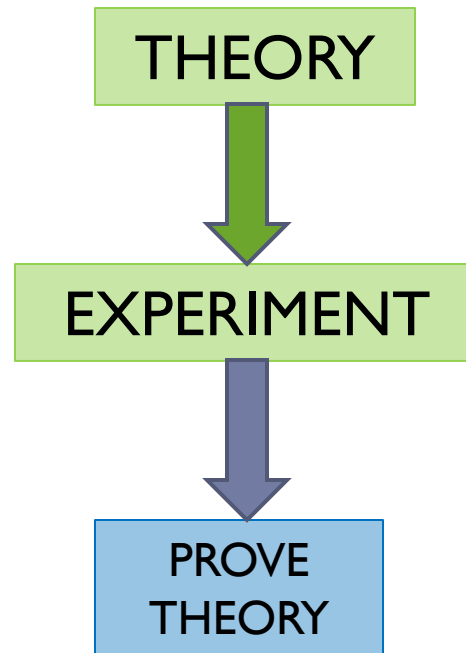
"We cannot understand the universe if we do not first learn the language and grasp the symbols in which it is written... it is written in the mathematical language"

Galileo



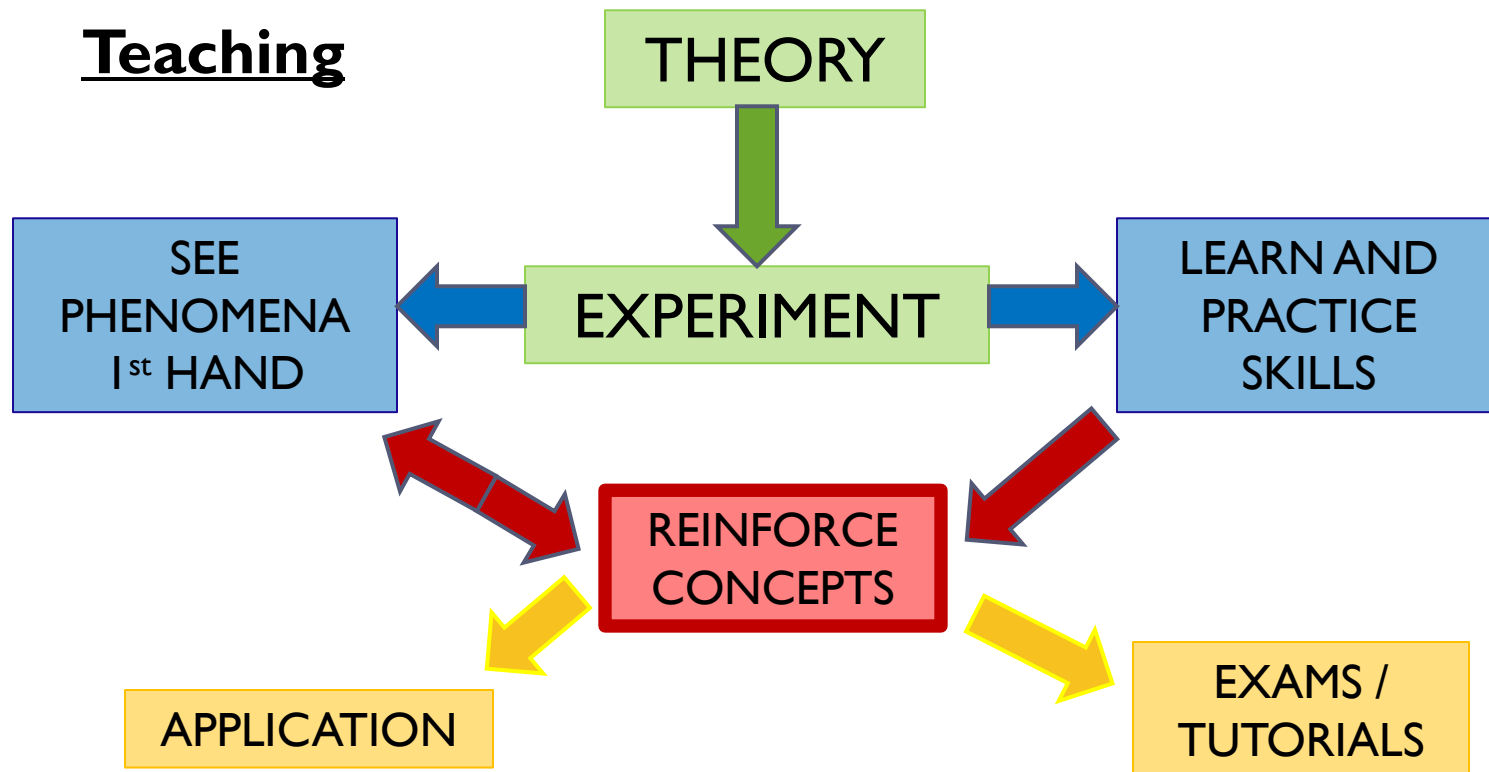
# Scientific Method in Research

## Research





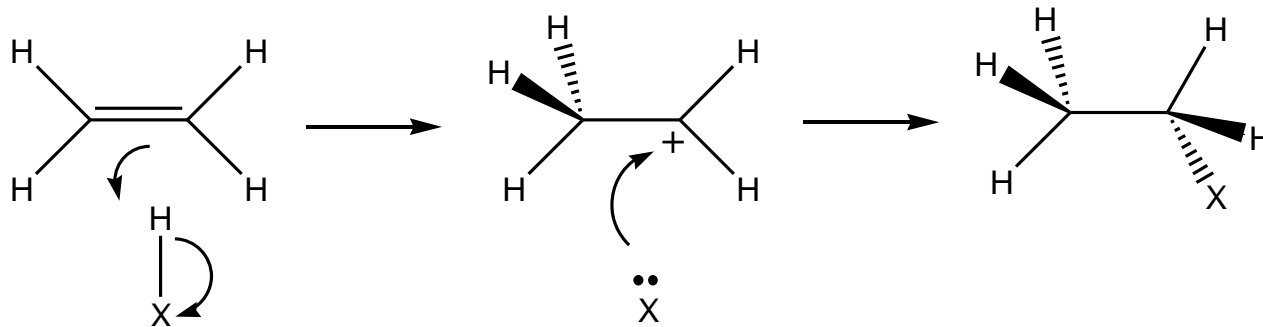
# Scientific Method in Teaching





# Chemistry Example

- ▶ Lectures might give a general mechanism



- ▶ Teaching laboratory experiment allows students to practice using it (methods, reagents, conditions), and reinforce the mechanism
- ▶ May also help the students to discover
$$\text{HF} < \text{HCl} < \text{HBr} < \text{HI}$$
- ▶ And the determine why this should be the case



# Staged Learning

- ▶ Theory
- ▶ Experiment
- ▶ Deeper understanding



- ▶ However, we do not have this staged learning in Chemistry for mathematical models
  - ▶ Just theory
  - ▶ Then some questions
    - ▶ No consolidation through useful practice, despite plethora of research level tools
    - ▶ Difficult to see the real ideas
- ▶ When Chemists discuss modelling, they think of...



# Chemical Modelling





## Problems for (Chinese) Chemists

- ▶ Chemists often a little afraid of maths and ignore the physics
  - ▶ So modelling is very uncommon
- ▶ Do not link ideas from separate lecture courses (physics, thermodynamics, statistical mechanics etc.)
  - ▶ Need to be more holistic in their approach
- ▶ Research software uses UNIX interface - very alien
- ▶ Most do not have programming experience



# Objectives

- ▶ Teach students how to think using models, and apply this knowledge to real chemical phenomena
  - ▶ Simplicity, power and scalability of classical physics
  - ▶ Do not fear maths
  - ▶ See the applications of abstract concepts
- ▶ A feel for modelling
  - ▶ Which models to use when
  - ▶ Balance of complexity versus accuracy
    - ▶ Models
    - ▶ Size
  - ▶ No model is perfect!



## Lecture - concept

- ▶ Want to teach students to connect microscopic and macroscopic to get bulk properties

### Microscopic

- ▶ Atomic mass
- ▶ Atomic charge
- ▶ Molecular geometry
- ▶ VDW parameters

### Macroscopic

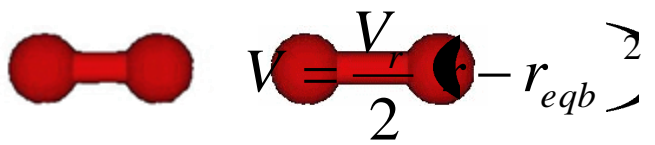
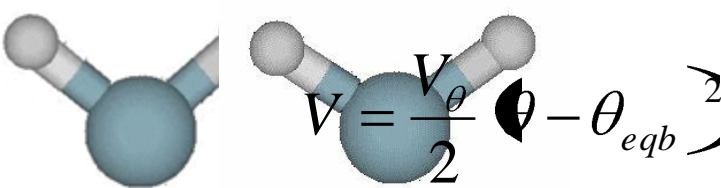
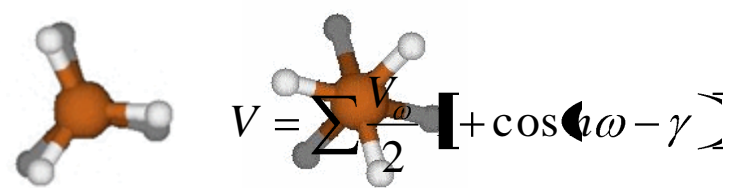
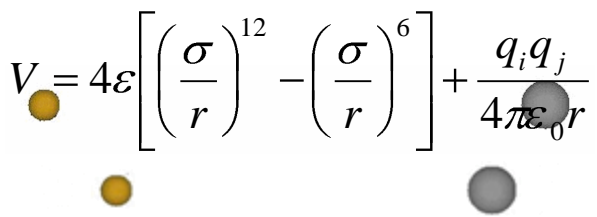
- ▶ Density
- ▶ Compressibility
- ▶ Heat capacity
- ▶ Viscosity
- ▶ Chemical potential



## Lecture - concept

- ▶ Want to teach students to connect microscopic and macroscopic to get bulk properties
- ▶ The question is then, how to think about the microscopic properties?
  - ▶ Chemists are taught from high school to think of molecules as balls connected by sticks
  - ▶ This corresponds to the idea of classical forcefields
    - ▶ Balls of a given mass attached by springs
    - ▶ Modelled using classical physics like Hooke's law

# Lecture - model

 <p style="text-align: center;"><math>V = \frac{V}{2} (r - r_{eqb})^2</math></p> <p style="text-align: center;">Bond stretching</p>	 <p style="text-align: center;"><math>V = \frac{V}{2} (\theta - \theta_{eqb})^2</math></p> <p style="text-align: center;">Angle bending</p>
 <p style="text-align: center;"><math>V = \sum \frac{V}{2} [1 + \cos(n\omega - \gamma)]</math></p> <p style="text-align: center;">Torsional interaction</p>	 <p style="text-align: center;"><math>V = 4\epsilon \left[ \left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^6 \right] + \frac{q_i q_j}{4\pi\epsilon_0 r}</math></p> <p style="text-align: center;">Non-bonded interaction</p>



## Lecture – statistical mechanics

- ▶ The more configurations we look at, the better the average
- ▶ The probability of the system having an energy state  $E_i$  is given by the canonical distribution (already explained in lectures)

$$p_i = \frac{e^{-E_i/k_B T}}{\sum e^{-E_j/k_B T}}$$



## Lecture – Newton

- ▶ Things move according to the forces on them

$$F = ma$$

- ▶ The forces can be calculated from the potential energy

$$F = -\frac{dV}{dx}$$



# Computer Lab

## Monte Carlo

- ▶ Generates a lot of configurations according to a canonical distribution

## Molecular Dynamics

- ▶ Generates a lot of configurations according to Newton's laws

- ▶ Then take averages (ensemble averages) of properties at the end



# Computer Lab

- ▶ Give a work sheet with
  - ▶ Summarised theory and explanation of the models
  - ▶ Instructions
- ▶ Computer with installed software and student demonstrator
- ▶ Leave them to it
  - ▶ Let them play around with it
- ▶ Outputs....
  - ▶ Compare to experimental results
  - ▶ Why is it different?
    - ▶ Analysis of the pros and cons of each model
    - ▶ Computer time vs. accuracy



## Computer Lab – The trick

- ▶ The ideas of MC/MD are relatively simple
- ▶ The difficulty lies in:
  - ▶ The interface – UNIX is the standard for these tools but it can be intimidating for new users
  - ▶ The input files – these have very specific formats with some quite technical parameters
- ▶ The simple solution is to provide a much simplified interface
  - ▶ i.e. a short program to ask for some general parameters and then write files / run the MC automatically
- ▶ Also, must use expertise to carefully choose test cases and avoid possible pitfalls



- ▶ **Need to prepare two macros:**
  - ▶ One to set up the input files
    - ▶ System specifications
    - ▶ Forcefield
    - ▶ Configuration
    - ▶ Then run the program
  - ▶ One to analyse to output
    - ▶ Extract the final answer
    - ▶ Calculate desired properties
    - ▶ Possibly write a molecular trajectory



# Tutorial

- ▶ The lab session has experimental (NIST) data to compare for each computer experiment
  - ▶ The students must explain differences between experiment and simulation
  - ▶ Also compare different models and differences in results
- ▶ Reinforce key objectives...



# Outcome

- ▶ Understand the principals of modelling
  - ▶ What is the problem?
  - ▶ What model is appropriate?
- ▶ Show classical physics
  - ▶ Still has a place in research
  - ▶ Can be used to calculate useful properties
  - ▶ Is not difficult to use
- ▶ Provide real applications to reinforce learning



## Good and Bad

- ▶ These programs are free
- ▶ Can give students a pretty easy introduction to modelling on a research level
- ▶ Shows the USE of these ideas – a big source of encouragement for the students to learn it better

But...

- ▶ Interface is still a little tricky
  - ▶ Could use java interface, but would be misleading
- ▶ Needs an experienced person to set it up



# Summary

- ▶ Modelling concepts are difficult for Chemists
  - ▶ Not supported by experiments
- ▶ Simple modification of research level programs can be made
  - ▶ Gives students chance to use modelling
  - ▶ Reinforce learning
  - ▶ Better Chemists

# Future

- ▶ Tested with masters students (due to English level)
  - ▶ Understanding is better and can explain pros and cons of models
- ▶ Possibly extend this to other lecture courses
  - ▶ Organics chemistry for optimised structures
  - ▶ Thermodynamics – equations of states for mixtures



Thanks for your attention

"I cannot teach anybody anything, I can only make  
them think." -- Socrates