

CHEM2524/2924/2534
Chemical Physics

THE UNIVERSITY OF SYDNEY

COMMONWEALTH OF AUSTRALIA

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Your Lecturers

Weeks 1-4 & 13
Lectures 1-11 & 37-39



Dr Wesley Dose
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Weeks 4-8
Lectures 12-25



A/Professor Toby Hudson
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Weeks 9-12
Lectures 26-36



A/Professor Asaph Widmer-Cooper
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Course Overview

- Lecture 1 The Role of Models
- Lectures 2-6 Stability, Symmetry and Structure of Matter
- Lectures 7-8 Bonding and Electron Delocalisation in Materials
- Lectures 9-11 Electronic, Dielectric and Magnetic Properties of Materials
- Lectures 12-17 Statistical Mechanics
- Lectures 18-19 Defects
- Lectures 20-23 Thermodynamics
- Lecture 24 Kinetics of Phase Transitions
- Lecture 25 Glasses
- Lectures 26-29 Soft Matter
- Lectures 30-31 Liquids
- Lectures 32-36 Surfaces
- Lectures 37-39 Metal-Organic Framework Materials

Assessment

Weekly Quizzes (10%)

- Early feedback task in week 3 (1%)
- 10 quizzes (1% each, discard worst result), to be held in weeks 1, 2, 4, 6, 7, 8, 9, 10, 12 & 13.
- You can repeat these as many times as you wish.
- To be completed on-line before the end of each Sunday (11:59 pm).

On-line Tests (10%)

- 2 of these (5% each), to be held in weeks 5 & 11.
- 15 questions, 1 hour time limit.
- To be completed on-line before the end of each Sunday (11:59 pm).

Exam (55%)

- In normal exam period.

Lab - Chem2x24 (25%) / Workshop - Chem2534 (25%)

Quiz Instructions

This pre-lecture quiz is open until 23:59 Sunday Week 1.

These are mastery quizzes: we want you to master this material and you can have as many attempts as you like. Your highest mark will be recorded. Truly mastering the concepts will lead to many more marks in the tutorial quizzes and exam than each mastery quiz is worth.

Question 1 — 1 pts

The flag of Australia has the following symmetry elements:



- ○ Mirror plane (2D point group: D1)
- ○ Two-fold rotation axis/inversion symmetry (2D point group: C2)
- ○ No symmetry (2D point group: C1)
- ○ Two-fold rotation axis/inversion symmetry, vertical mirror plane, horizontal mirror plane (2D point group: D2)
- ○ Four-fold rotation axis, two-fold rotation axis/inversion symmetry, vertical mirror plane, horizontal mirror plane, two diagonal mirror planes (2D point group: D4)

Question 2 — 1 pts

The flag of Cambodia has the following symmetry elements:



- ○ Two-fold rotation axis/inversion symmetry (2D point group: C2)
- ○ Mirror plane (2D point group: D1)
- ○ Two-fold rotation axis/inversion symmetry, vertical mirror plane, horizontal mirror plane (2D point group: D2)
- ○ No symmetry (2D point group: C1)
- ○ Four-fold rotation axis, two-fold rotation axis/inversion symmetry, vertical mirror plane, horizontal mirror plane, two diagonal mirror planes (2D point group: D4)

Question 3 — 1 pts

The flag of Switzerland (1:1 aspect ratio version) has the following symmetry elements:

Canvas

Weekly pages

Unit info & Schedule

Assessments

Staff contacts

University student support

- https://www.sydney.edu.au/students/support.html

The School of Chemistry needs you!

Staff-Student Liasson Committee (SSLC) Student representatives

Purpose: Collate student feedback so we can keep improving your learning experience.

Benefits: Academic engagement, CV enhancement and free lunch!

- We meet twice a semester over lunch
- *Interested*? Contact your unit lecturer or Dr Pierre Naeyaert by end of Week 1.



Chair of the Staff-Student Liaison Committee:

Dr Pierre Naeyaert

Room 457, School of Chemistry (F11)

pierre.naeyaert@sydney.edu.au

The Role of Models

Lecture 1

Unit Outline

Role of Models

Models and Mathematics

Classical vs Quantum

Lecture 2

Interparticle Interactions

Molecular Symmetry

Introducing Models

A **model** is a representation of some aspect of the natural world, sufficiently simplified to be intelligible while still effectively capturing some aspect of reality.

By this definition, maps are models – the maker of each map has chosen details to keep and details to omit.



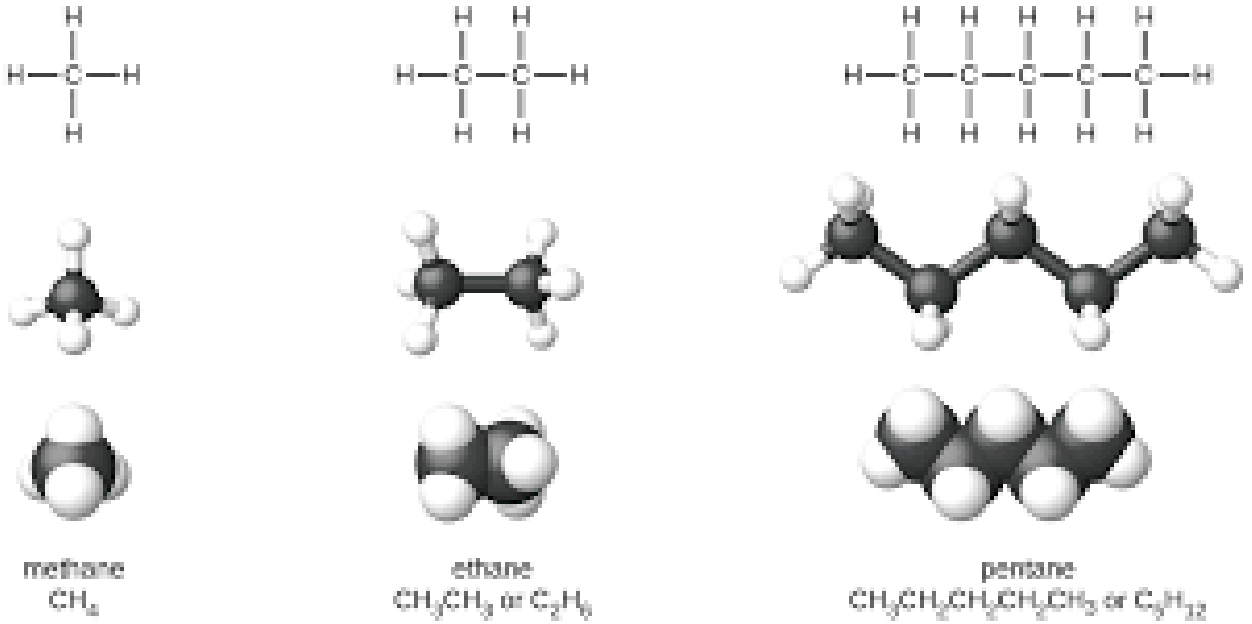






We judge the usefulness of a map in terms of the task it was designed to perform

Models in Chemistry



Different types of models

Connectivity

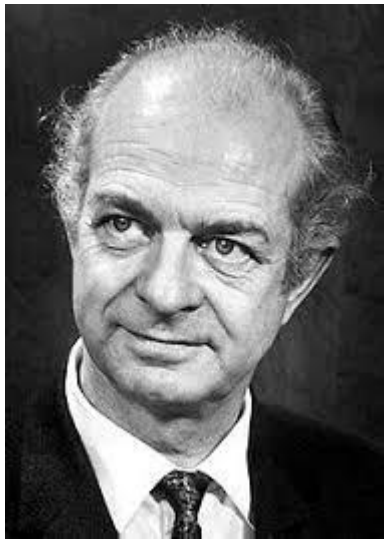
Connectivity + bond angles

Connectivity + bond angles + filled space

Notice that models don't have to be physical objects. They can exist just on paper or even just as ideas.

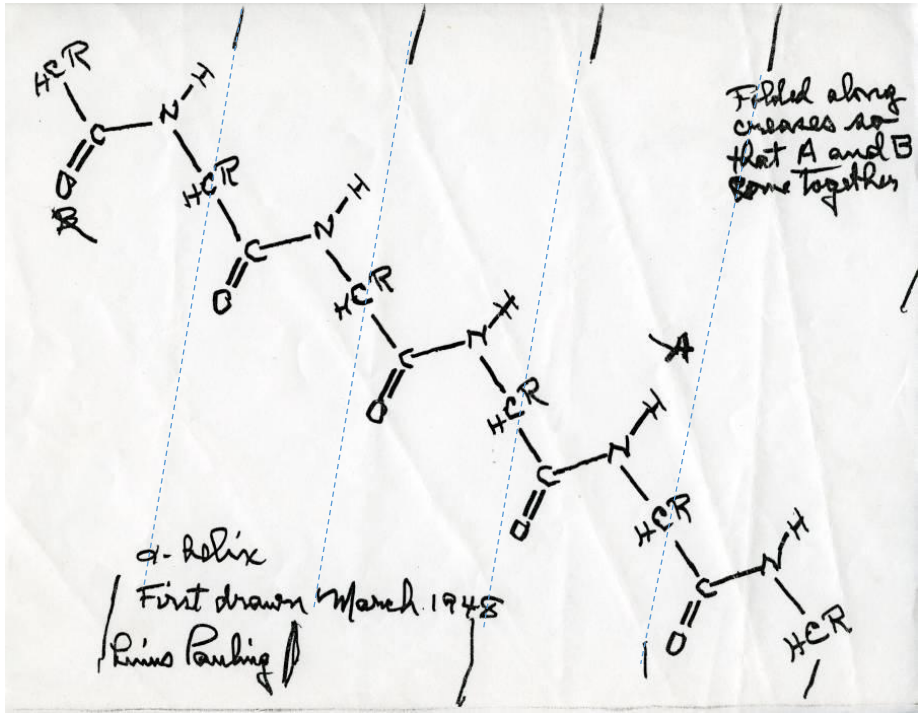
https://en.wikipedia.org/wiki/Heuristic

Discoveries can be made by manipulating models

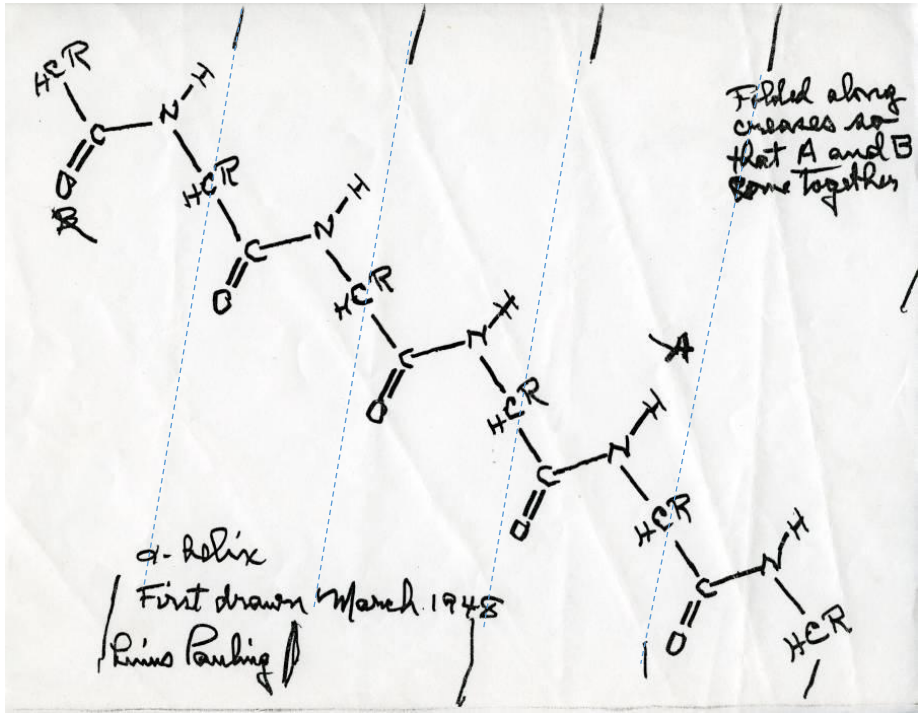


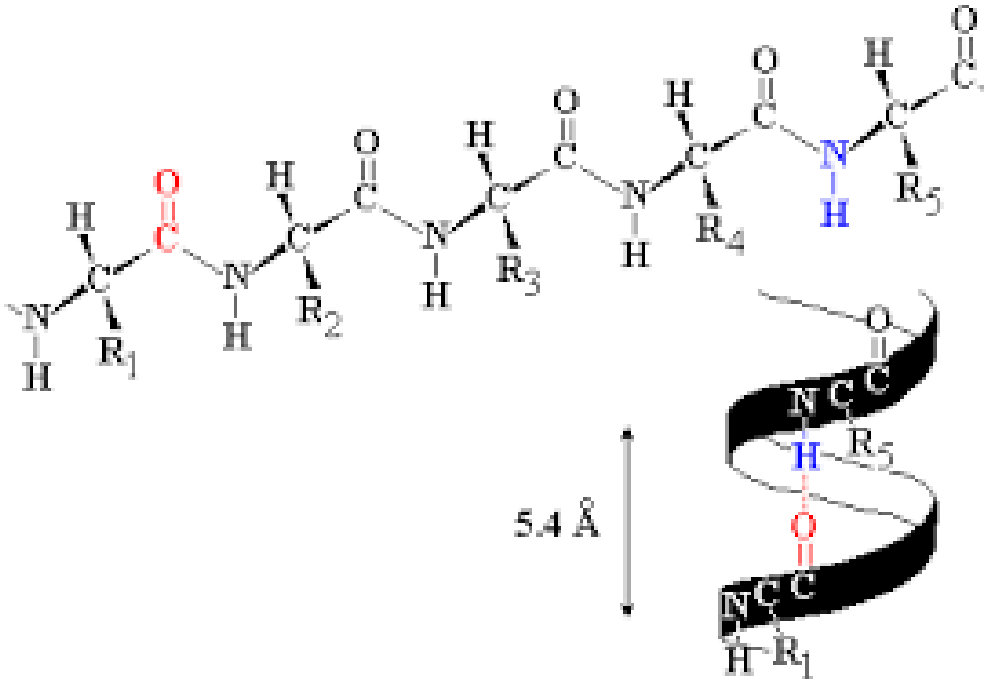
In 1948, Linus Pauling was stuck in a London hotel with a cold and thinking about the structure of a simple protein chain

He drew this structure on a sheet of paper and folded along the dotted lines to model the tetrahedral geometry of these carbons



Discoveries can be made by manipulating models





The prediction was the α helix structure of proteins – the principal geometry in hair, horns and nails and also present in all globular proteins like enzymes

The α helix structure of a protein

The Watson-Crick structure of DNA relied on models to establish that the base pairs would fit



Watson and Crick after predicting the double helix structure of DNA 1953



Their result was in the form of this physical model



The crucial observation – that paired bases could fit inside the double helix – was made using models of the bases like these

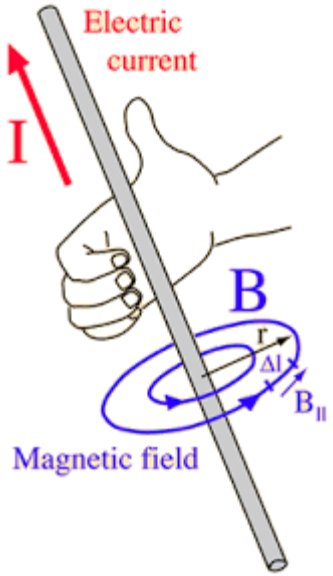
Models and Understanding

What do we mean when we say we *understand* something?

I never satisfy myself until I can make a mechanical model of a thing. If I can make a mechanical model I understand, I can understand it.

William Thomas (Lord Kelvin) 1884

An Example of Modelling



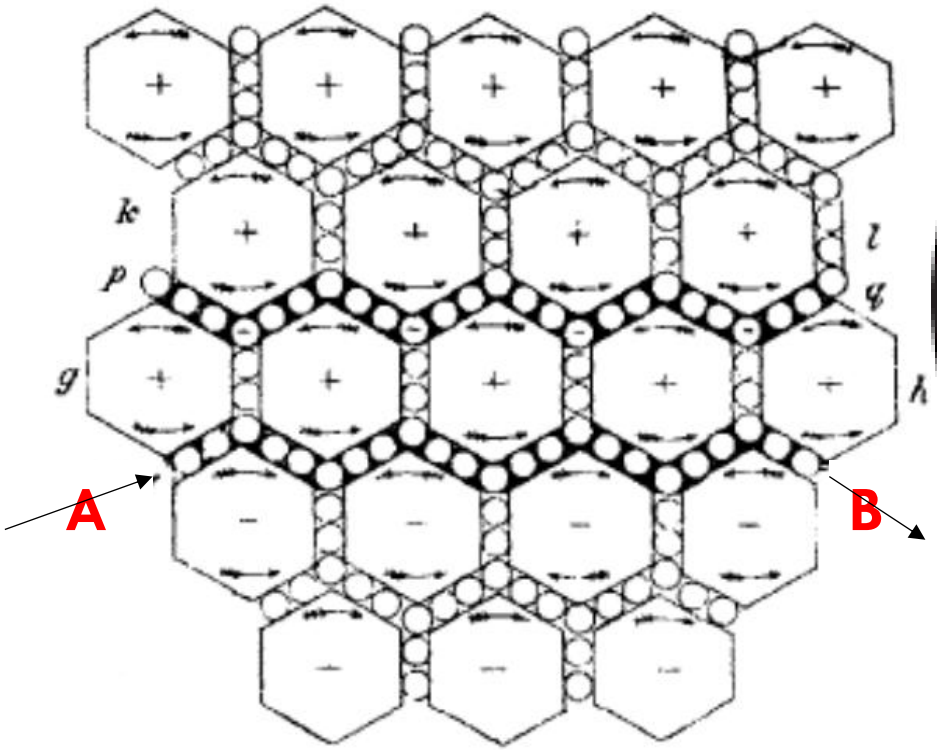
Ampere had observed that a moving current induces a magnetic field.

Maxwell set out the 'explain' this connection between current and magnetic field using a mechanical model.



James Clerk Maxwell 1863

Models and Understanding: Maxwell's Model

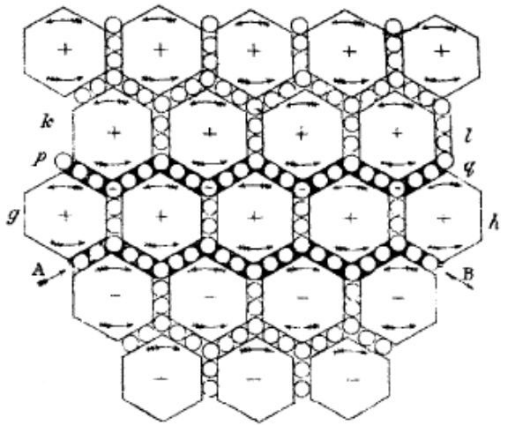


Electric current flowing from A to B is represented by sliding the line of small "wheels". As they move, they set in motion the vortices (hexagons) – clockwise below (a – sign) and anticlockwise above (a + sign). The angular velocity of these vortices represents magnetic force. And so the current has induced a magnetic field satisfying the right-hand rule! QED



Models and Mathematics

Maxwell quickly replaced his model of vortices and wheels with mathematical expressions that captured the same behaviour – without all the extraneous bits of invention, i.e.



=

$$\nabla \cdot \mathbf{E} = \frac{\rho}{\varepsilon_0}$$

$$\nabla \cdot \mathbf{B} = 0$$

$$\nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

$$\nabla \times \mathbf{B} = \mu_0 \mathbf{j} + \frac{1}{c^2}\frac{\partial \mathbf{E}}{\partial t}$$



Mathematical expressions represent the most compact and unambiguous expression of the relations between quantities and, implicitly, the physical mechanism by which they are connected – i.e. **maths is a language for precisely defining a model**

Mathematical expressions are also a convenient tool for quantitative predictions.

General Modelling Strategies: Dimensional Analysis

Physical phenomena are typically characterised by one or more length scales and energy scales.

Scaling and Back of the Envelope estimates are the best place to start in modelling.

Example 1 How plausible is Giant-Man (aka Ant-Man)?

If L is the dimension of an object, the mass $\propto L^3$

The strength of bones is proportional to the cross-section area A, so A must increase with the mass, i.e., with L^3, to ensure an object doesn't break under its own mass.

Expanding each dimension by the same scale, as is the case for Giant Man, increases A by L^2.

Conclusion: Giant Man's mass would crush his bones.



We can often answer our questions using this kind of simple scaling analysis.

https://profmattstrassler.com/2022/06/21/dimensional-analysis-a-secret-weapon-in-physics/

General Modelling Strategies: Dimensional Analysis

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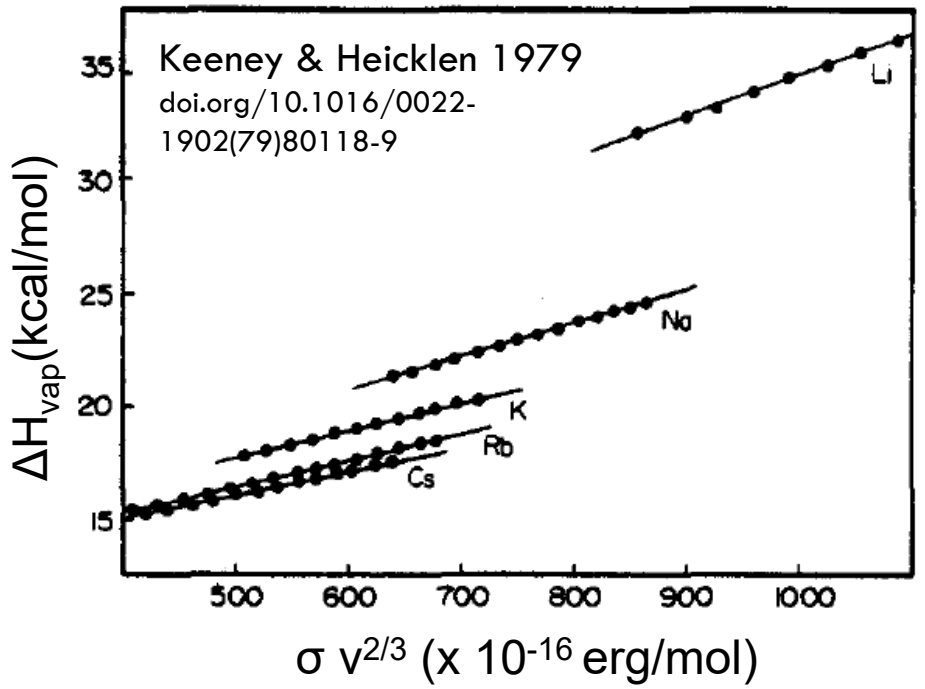
Example 2 How does a liquid's surface tension change with temperature?

Surface tension σ has units of energy/area.

The energy to create a surface should be $\propto \Delta H_{vap}$, the enthalpy difference between liquid and vapour.

The area, A, should scale with the volume, v, occupied by a molecule. Since $A \propto L^2$ and $v \propto L^3$, then $A \propto v^{2/3}$.

Therefore, ΔH_{vap} (y-axis) $\propto \sigma\, v^{2/3}$ (x-axis) resulting in the straight-line relationship in the graph.



Quantum or Classical Mechanics?

Classical mechanics describes the world as trajectories (i.e., positions and velocities) – e.g., tracking airplanes in the sky.

Quantum mechanics describes the world as wave functions (i.e., time dependent amplitudes distributed over space) – e.g., an electron in an orbital.

Generally, trajectories are much easier to work with than wave functions (and computationally less expensive).

When is classical mechanics a reasonable approximation?

A question of length scales: The spatial extent of a wave function is the de Broglie length

$$\lambda = h/p$$

Planck's constant $h = 6.626 \times 10^{-34}$ Js and p = mass x velocity (i.e., the momentum)

Classical mechanics is valid when $\lambda \ll$ the characteristic length of the phenomena

Quantum or Classical Mechanics?

	de Broglie length $\lambda = h/p$		relevant length	classical or quantum?
Electron in a H_2 molecule	3.3×10^{-10} m	>	7.4×10^{-11} m (H-H bond length)	quantum
Liquid argon at T = 80 K	0.9×10^{-10} m	~	1.8×10^{-10} m (atomic radius)	?
C_{60} at T = 273 K	4.0×10^{-12} m	<	0.7×10^{-9} m (C_{60} diameter)	classical

Classical mechanics can generally be used except when dealing with small momenta – i.e., low mass particles (electrons, photons, protons) and/or very low temperatures.

Role of Computers in Modelling

Do you understand a phenomenon? Computer modelling provides a litmus test of how well you are doing.

If you had as much computer capacity as you wanted, could you explain to a computer (i.e., write an algorithm) how to model the phenomenon?



- Boiling of a simple liquid can be simulated and satisfactorily predicted by theory.



- Liquid turbulence can be simulated even though we still do not have a theory for complex flows.



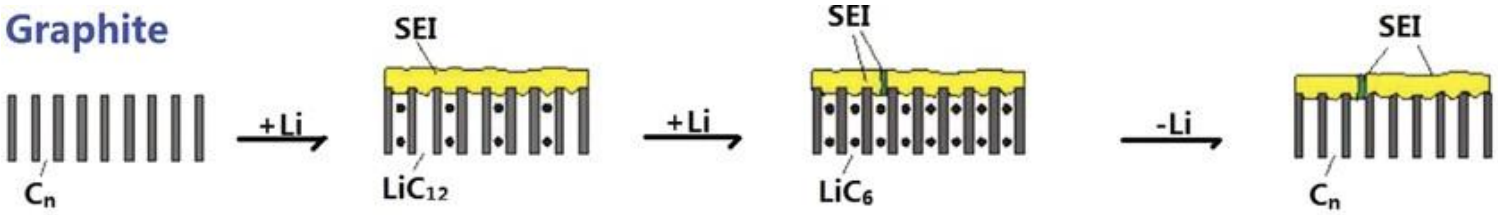
- High temperature superconductivity cannot yet be reproduced in a computer simulation.



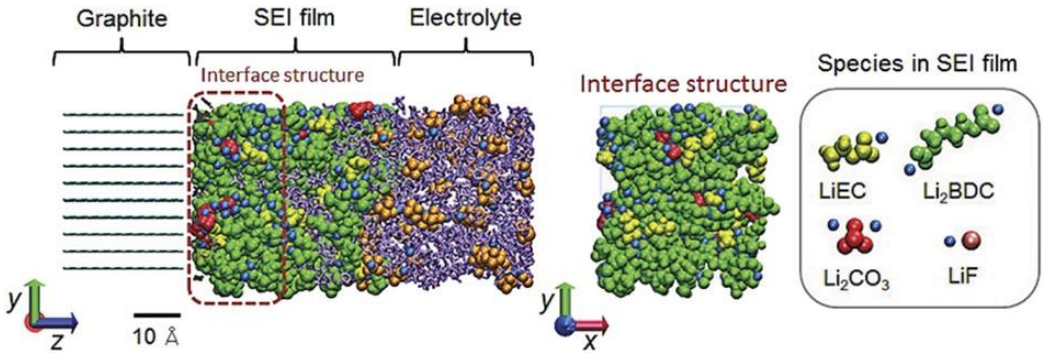
Increasing computational challenge = conceptual difficulty

Case study: Modelling of the solid electrolyte interface (SEI) for lithium-ion batteries

An interfacial layer forms on the graphite particle surface due to electrochemical reduction of the electrolyte. Termed the SEI, it allows Li^+ transport and blocks electrons, enabling the battery to store/release energy.

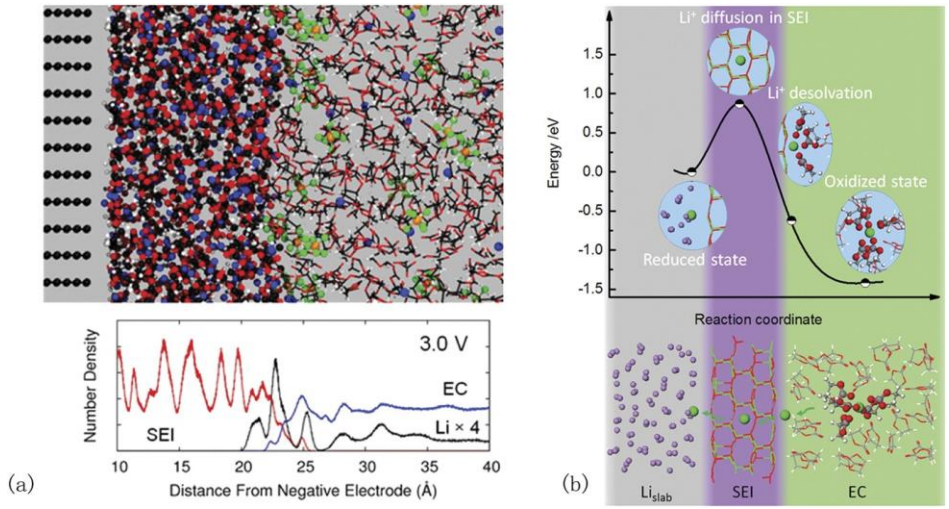


The SEI forms with structural and compositional heterogeneity at the nanoscale and evolves over time.



https://www.nature.com/articles/s41524-018-0064-0
https://www.sciencedirect.com/science/article/pii/S2542435119304210

Limited understanding of its chemical/structural properties make it challenging to model processes in the battery, e.g., ion transport.



Learning Outcomes

After this lecture you should be able to

- Understand the sequence of topics covered in this unit.
- Appreciate what a model is and the role modelling plays in science.
- Understand the relation of mathematics and computer-based calculations to how molecules are developed and used.