University of Sheffield

Materials -
a SUBJECT
that MATTERs

Dr Colin Freeman

Materials Simulation

Jurassic Park

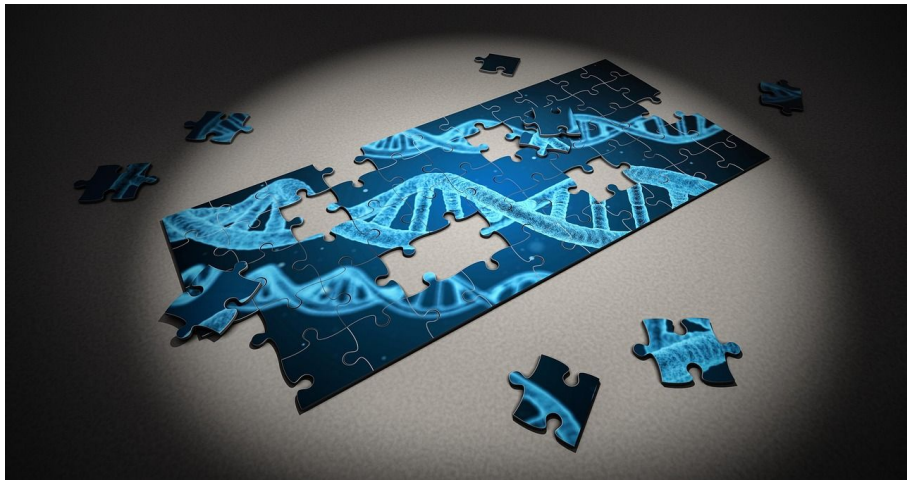
Did it even exist?

What is Materials Science and Engineering (MSE)?

MSE is defined as an ‘interdisciplinary subject, bridging the physics and chemistry of matter towards engineering applications and industrial manufacturing processes.’ The programme content spans from foundations in physics and chemistry to the mechanical, electrical, magnetic, and optical properties of materials, and the design, manufacture and applications of metals, alloys, ceramics, polymers, composites, and biomaterials.

MSE continues to establish itself amongst engineering disciplines and is offered as a degree course across the UK at the Universities of Birmingham, Cambridge, Imperial College London, Leeds, Loughborough, Manchester, Oxford, Queen Mary, Sheffield and Swansea, as well as Materials Chemistry being offered at St Andrews and Glasgow.

Key Learning outcomes



- **What is DNA?**
  DNA is often referred to as the instruction manual for living organisms. The cells in our body all contain our unique genetic code in our DNA and this is how successful traits are passed onto future generations.

- **Why is it important to understand the decay process of DNA?**
  Whenever an organism dies it will leave behind its DNA. This DNA can lose its shape over time and undergo chemical reactions with the environment leading to the sequence of the bases being broken up. How readily the DNA undergoes these reactions depends on the environment it is in.

  This decay may result in the DNA no longer storing the genetic information correctly and data can be lost, therefore, understanding what affects this decay and what happens to DNA molecules over time is important.

- **How does modelling and computer simulation accelerate the research into DNA?**

  Scientists like Dr Freeman can perform simulations of DNA molecules in solutions and on the surfaces of minerals.

  These simulations can identify how molecules bind to surfaces and how this can change the structure of the molecule. This tells us if the molecule is more likely to break apart or not. His research has identified that DNA will bind to certain mineral surfaces, and this may protect it from being broken apart, enabling it to last longer.

  How molecules bind onto material surfaces can affect a lot of other areas. Bacteria will use molecules (DNA in particular) to bind to material surfaces. As bacteria builds up on a surface biofilms are formed causing problems in a range of systems – water pipes, food processing, medical equipment – where the bacteria leads to infection and disease. If we can understand how these molecules bind then we can look at making materials which inhibit this binding and stop bacteria growing.

GCSE Chemistry topics this episode could be taught alongside…

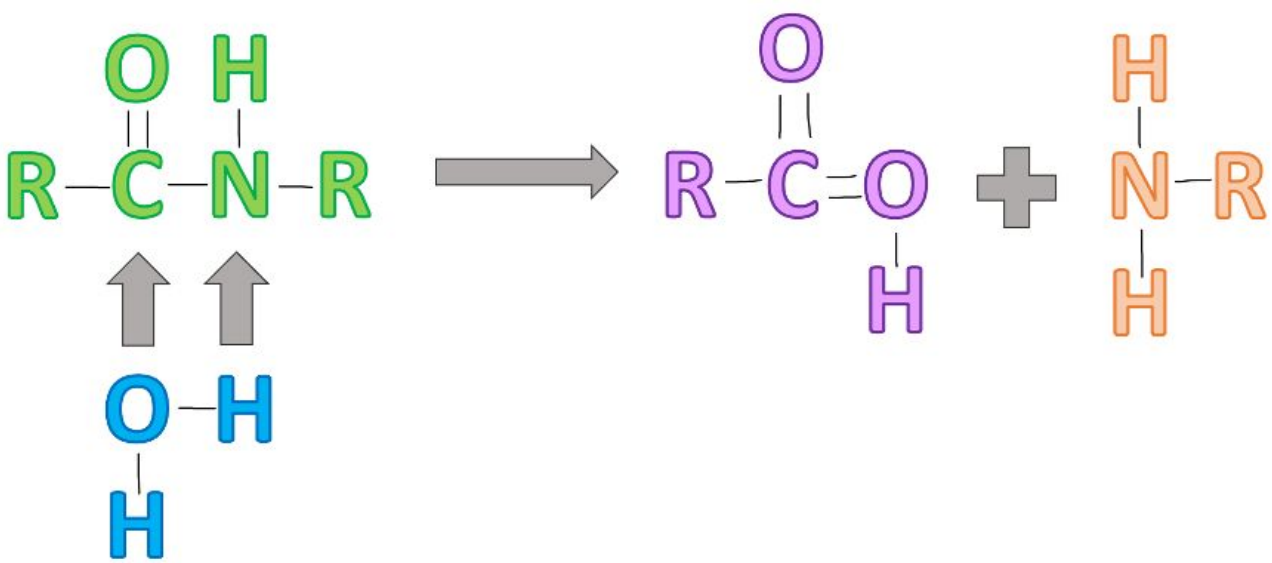
Organic Chemistry	Polymers (DNA and Natural Polymers)	Condensation and Natural Polymers

How does this episode go beyond the curriculum?

In both chemistry and biology students learn the basic definition of DNA…

In GCSE chemistry students learn about the **hydrolysis** reaction which involves heating an ester and molecules, including DNA decay over time via hydrolysis.

Hydrolysis is the process in which water reacts with the bonds holding the peptides (and other molecules) together. The molecules are then broken apart and lost.



DNA and the double helix structure

Due to the structure, parts of the DNA will decay quicker, and parts of the DNA will last longer.

People have been mistaken in thinking that the part of DNA that has survived the longest must be the most important part of the genetic code for that molecule, however it is simply the part that takes the longest to decay!

The vulnerable groups and parts of the DNA molecule that are the most susceptible to decay are inside the double-helix…

Lots of Europe rests on calcite and other carbonate deposits laid down millions of years ago e.g., the Yorkshire Wolds and the oil fields of the north sea.

This is because DNA binds strongly to the calcite surface.

DNA binding involves pulling the bases out of the helix structure which leads to a break up of the molecule. DNA will then become more vulnerable to hydrolysis and so the lifetime of the molecule is reduced.

Key definitions

DNA

DNA stands for deoxyribonucleic acid.

DNA is a chemical made up of two long strands, arranged in a spiral.

This is known as the double-helix structure.

The molecule carries genetic information in the form of genetic code.

Evolution

The process by which different kinds of living organism are believed to have developed from earlier forms during the history of the earth.

Evolution is seen as a change in the inherited characteristics of a population over time through natural selection.

This process may also result in the emergence of new species.

Horizontal gene transfer

A process that enables rapid evolution between organisms through the transfer of genetic matter.

When DNA is released by a dead organism into the environment, another organism may consume this DNA and that material might be used and enter its genetic matter.

Computer modelling and simulation

A physical or logical representation of a given system which can then be used to generate data.

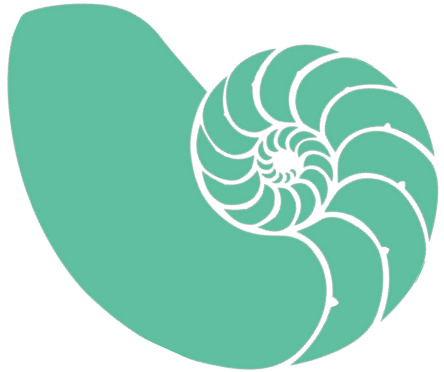
This can help to make decisions or predictions about the system.

Questions to think about...

From the episode can you remember how old the longest surviving DNA is so far?

The longest surviving DNA that has been identified so far is about 2 million years old. Dinosaur DNA would be from 65 million years ago and so this suggests that Jurassic Park cannot be real!

Certainly, Dr Freeman's research suggests it would not survive very long in a fossilised mosquito!



How does horizontal gene transfer help explain evolution?

At the very early stages of life on earth there are a lot of questions about how evolution progressed, and genetic matter was transferred between organisms.

When DNA is released by a dead organism into the environment another organism might consume this DNA and that material is likely to be used and enter its genetic matter.

If the DNA decays, is broken apart and loses it's sequence then genetic information would not pass across to the new organism.

However, DNA that sticks onto a mineral surface will survive longer without decaying and this DNA has a greater chance of entering another organism.

Discussion Topics…

What materials are made in the natural world by living creatures?

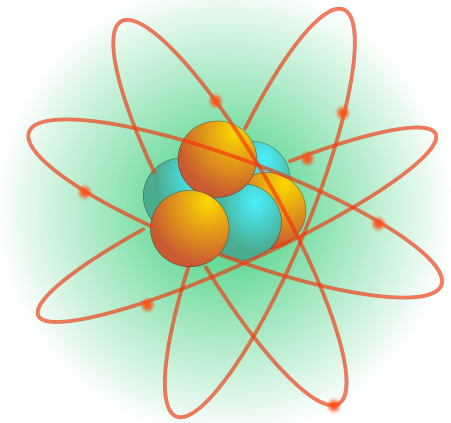
- Teeth
- Bone
- Shells
- Wood
- Sand
- Rocks
- Soil
- Chalk
- Silks and natural fibres

Why are researchers simulating the existence of natural materials if nature can simply make them for us?

Natural materials such as biominerals like shells and teeth are made up of crystals which have structures made up of complex shapes.

These shapes are too complex for scientists to accurately replicate the structure of the material in the lab, and so we can simulate the interaction of these complex natural materials instead to understand how they would behave and interact in different situations.

Discussion Topics…



What is a classical simulation to study?

We can study atomistic simulations.

Molecules and crystals are collections of atoms and ions (you can imagine these as lots of balls being pulled and stuck together by lots of forces!).

As studied at GCSE, basic force equations for objects such as

FORCE=MASS X ACCELERATION

can be used in a model to simulate and calculate the basic movement of the atoms under those forces.

Additional Resources

- **Horizontal gene transfer, stated clearly video**
  https://www.youtube.com/watch?v=BiRc2FGh71o

- **Making Fossils Science practical**
  https://www.preproom.org/practicals/pr.aspx?prID=1048

- **The Guardian article- Reality bites: ‘Could Jurassic Park actually happen?’**
  https://www.preproom.org/practicals/pr.aspx?prID=1048