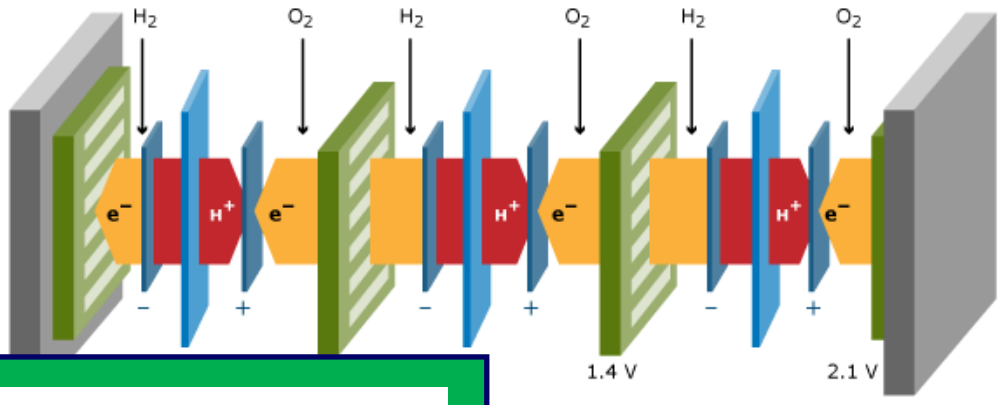
Green Machines-Hydrogen Fuel Cells for the Future's Cars

2016-2017

Tutor Name Jane Yates



Student Name

Timetable and Assignment Submission

Fill this in with your teacher.

Timetable – Tutorials

Tutorial	Date	Time	Location
1			
2			
3			
4			
5			
6			

Timetable – Homework Assignments

Homework Assignment	Description	Due Date
Tutorial 1		
Tutorial 2		
Tutorial 3		
Tutorial 4		
Tutorial 5		

Assignment Submission – Lateness and Plagiarism

Lateness	
Submission after 4.00pm on **Friday 6th January 2017**	10 marks deducted
Plagiarism	
Some plagiarism	10 marks deducted
Moderate plagiarism	20 marks deducted
Extreme plagiarism	Automatic fail

The UniPathways – 2016/2017 – Pupil Feedback Report

Grade	Marks	What this means
1st	70+	Performing to an excellent standard at first year undergraduate level
2:1	60-69	Performing to a good standard at first year undergraduate level
2:2	50-59	Performing to an excellent standard at GCSE level
3rd	40-49	Performing to a good standard at GCSE level
Workings towards a pass	0-39	Workings towards a pass
Did not submit	DNS	No assignment received by Uni Pathways

Lateness	
Any lateness	10 marks deducted
Plagiarism	
Some plagiarism	10 marks deducted
Moderate plagiarism	20 marks deducted
Extreme plagiarism	Automatic fail

Name of PhD Tutor			
Title of Assignment			
Name of Pupil			
Name of School			
ORIGINAL MARK / 100		**FINAL MARK / 100**	
DEDUCTED MARKS		**FINAL GRADE**	

If marks have been deducted (e.g. late submission, plagiarism) the PhD tutor should give an explanation in this section:

Learning Feedback Comment 1	
What you did in relation to this Key Learning Priority	**How you could improve in the future**
Learning Feedback Comment 2	
What you did in relation to this Key Learning Priority	**How you could improve in the future**
Learning Feedback Comment 3	
What you did in relation to this Key Learning Priority	**How you could improve in the future**
Resilience Comment	
How you showed learning resilience during the course	**How you could build learning resilience in the future**

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Course Rationale

We all know that global warming is bad, air pollution is a problem and that petrol won't last for ever, so what kind of cars will we be driving in 50 years time? Is there a green way to solve our need for speed? This course aims to give students an insight into the world of fuel cells for cars. We'll be working from the point of view of a car manufacturer: assessing the green technology options for small vehicles; investigating at the latest developments in fuel cell technology and looking at how computer modelling is used to develop even better fuel cell components.

Over the course of the sessions students will interact with scientific journals to develop their information retrieval skills, critically assess the best catalysts in development and use their creativity and newly gained scientific knowledge to suggest possible avenues for research and development.

Following an initial introduction to the different green energy options being explored for vehicles: green fuels, batteries and fuel cells, students will learn the chemical and electrochemical concepts behind hydrogen fuel cells. Once familiar with fuel cells and how they work, we will progress to consider possible ways to improve the fuel cell catalysts to boost energy production. The use of computer modelling to explore reactivity and support experiment will also be explored. The course will culminate in a research and development exercise in which the students will assess real data and propose research plans for the next generation of hydrogen fuel cell catalysts.

Mark Scheme

Key Skill	1st	2.1	2.2
Data Analysis	☐ Interpretations of graphical data and numerical values are correct and well explained with reference to physical properties and processes discussed during the course ☐ Limitations of the data provided are discussed.	☐ Interpretation of graphical data and numerical values is attempted and generally correct. This is explained with some reference to the physical properties and or processes present. ☐ Limitations of the data are commented upon.	☐ Little interpretation of numerical values or graphical data is given. Where it is, the interpretation is often incorrect and little reasoning is given. ☐ Limitations of the data are not discussed.
Communication and Language	☐ Writing is clearly structured and flows logically. Headings are well chosen and employed throughout. ☐ Language use is accurate, and concise. There are very few (<5) spelling or grammar mistakes. ☐ The writing is of a style appropriate for a scientific report throughout. ☐ The technical vocabulary surrounding fuel cell performance and catalysis is well used throughout.	☐ The writing is structured with the use of suitable headings throughout. ☐ The language use is mostly accurate. Spelling and punctuation errors occur intermittently (5-15). ☐ The written style is mostly appropriate for a scientific report, however occasional lapses are evident. ☐ Moderate use of technical vocabulary is made and this is employed correctly in the majority of occasions.	☐ Writing is disjointed or often muddled. Headings are sometimes used but could be improved. ☐ Language is readable however the text includes frequent spelling and grammar mistakes (+15). ☐ Inconsistency in the written style results in a lack of clarity for the document as a whole. ☐ Technical vocabulary is rarely used or often implemented incorrectly.
Critical Thinking and Evaluation	☐ Critical evaluation of the data is systematic and logical. ☐ Data is discussed and compared and differences discussed. ☐ Conclusions are well reasoned and clearly drawn from the data. ☐ The final recommendations must be strong and draw together arguments from the whole report.	☐ Evaluation of the data is complete but unsystematic. ☐ The datasets are discussed and some comparison is made but this is incomplete. ☐ Conclusions are drawn from the data however the rationalisation could be strengthened. ☐ The final recommendations are clear and supported by the report.	☐ Some evaluation of the data is undertaken but this may be partial and unclear. ☐ Inconsistent evaluation of data sets and little comparison of data is seen. ☐ Conclusions may be weak and some reasoning incorrect. ☐ The student does provide a recommendation but it is only partially supported from the report assessment.
Research Skills	☐ A wide variety of reliable sources are used and are all referenced appropriately.	☐ A selection of mostly reliable sources are used and are references appropriately.	☐ Attempts to use sources are made and or attempts to reference are seen.

Glossary of Keywords

Greenhouse effect

Emissions

Particulate matter

Green energy

Biofuel

Battery

Fuel Cell

PEM

MEA

Anode

Cathode

Nafion©

Oxidation

Reduction

Catalyst

Overpotential

Finite Element

Molecular Dynamics

Density Functional Theory

Le Sabatier's Principle

Descriptor

Tutorial 1 – Green Machines: the Why and What?

What is the Purpose of Tutorial 1?

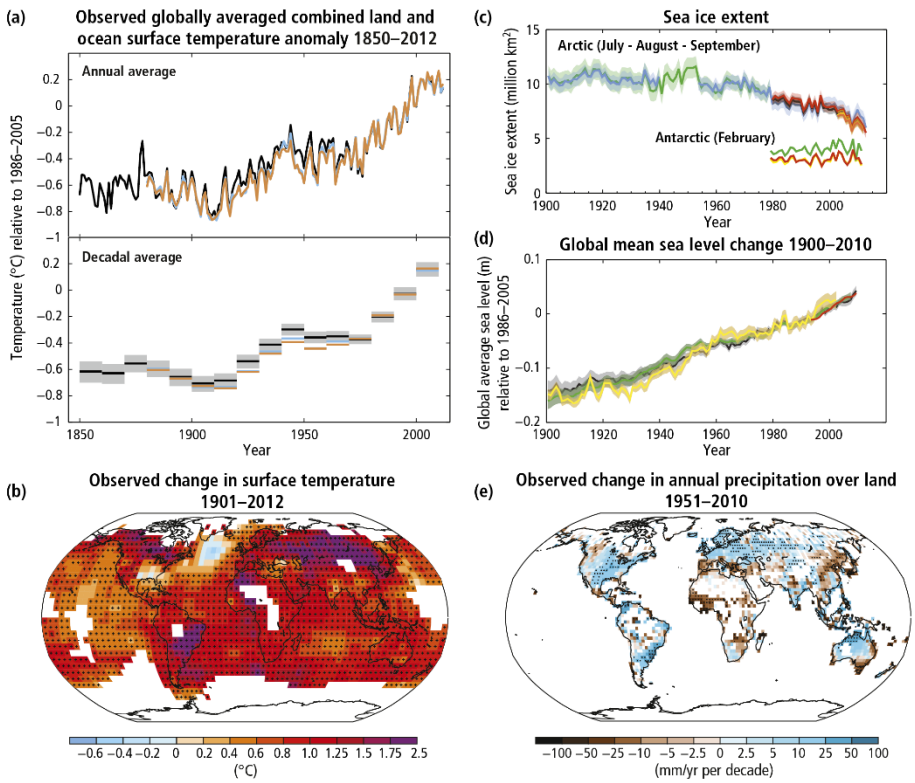
- To discuss what we know about climate change
- To consider the criteria the we'll use to evaluate our green energy options
- To introduce and contrast different green energy alternatives for small vehicles

Starter: What do we know about climate change?

What is it?

Causes?

Effects?



Key findings form the IPCC 2014 report on climate change

> **Fact Attack:** Did you know there is a difference between climate change and global warming? Climate change is occurring as a result of global warming: the trend of long-term global temperature increase. The greenhouse effect causes this rise in temperature.

- In 2008 the government passed the Climate Change Act: a long-term plan for the reduction of UK CO_2 emissions.
- By 2020 greenhouse gas emissions should be reduced by 34%.
- Domestic transport accounted for 24% of all UK emissions in 2009.

What criteria should car manufacturers use to choose their green energy strategy?

Activity 1- Green Energy Options

Use the information sheets provided to fill out the assessment grid for possible vehicle green energy sources. You may also find visiting www.nextgreencar.com helpful.

Green Energy Source	Advantages	Disadvantages
Bio-fuels		
Batteries		
Hydrogen Fuel Cells		

Tutorial 1 – Baseline Test

The homework assignment for the first tutorial is a baseline test to see your initial level of attainment in this subject area. The assignment will test for some or all of the subject specific skills that are required later in the final assignment. However, it is shorter than the final assignment and is will be an introduction to the subject as well as a challenge!

Do not worry too much about doing 'well' or 'badly' on the baseline test, it takes into account the fact that you may not be familiar with the subject area. It is designed to help you and your PhD tutor identify where you are at the start of the programme and to help you measure your progress along the way.

Using the information from Tutorial 1, write an evaluation of the green energy options for small vehicles. Please make a reasoned judgement as to which energy source you think has the greatest potential for the motor industry.

- **Present your findings as a summary report written for a technical audience.**
- **Aim to write in the region of 500 words (± 10%).**
- **Structure your findings with paragraphs and appropriate headings.**

Sources:

Biofuels: http://www.bp.com/en/global/corporate/sustainability/the-energy-future/biofuels.html
http://www.bp.com/en_br/brazil/o-que-fazemos/biocombustiveis/etanol-da-cana-de-acucar.html

Biofuels: the next generation

Gross, M. Biofuels the next generation. (2009) at <http://www.rsc.org/Education/EiC/issues/2009May/Biofuelsthenextgeneration.asp>

In Short

- Woody plant waste is converted to liquid oil by pyrolysis and then to syngas, opening up routes to a range of products normally made from petroleum
- Novel micro-organisms and enzymes are tailored to produce biofuels
- Algae biofuels do not compete with food crops for land use

First-generation biofuels made from carbohydrate-rich food crops, such as corn or sugar cane, have come under scrutiny as they compete with food crops for land use. Chemists are now turning their attention to dead wood, algae and genetically-engineered microorganisms to develop second-generation biofuels. *Michael Gross*

Climate change has risen to the top of the political agenda in recent years. Growing awareness of this problem has also raised the profile of fuels made from biomass - *ie* biofuels. Following the example of Brazil, which has used bioethanol as a transport fuel for many years, other countries have stepped up their production of fuels from carbohydrate-rich crops, such as corn or sugar cane. These fuels were initially seen as 'carbon neutral' because regrowing the crops would absorb the same amount of carbon dioxide as was released when burning the fuel. In 2003 the European Union set a target of replacing 5.75 per cent of all transport fossil fuels (petrol and diesel) with biofuels by 2010.

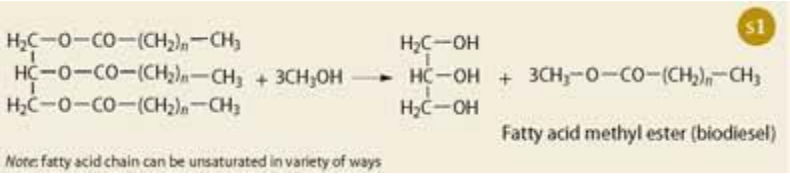
From food crops to agricultural waste

However, the increased production of such biofuels has quickly shown up their shortcomings. Fuel crops have begun to compete with food crops for land use and are already making food less affordable in developing countries. Furthermore, their green credentials have come under fire as the intensive farming methods required for efficient mass production of fuel crops use significant amounts of energy. By the end of 2007, it had become clear that the potential solution had become part of the problem.
Experts now pin their hopes on biofuels that are not produced from edible plant materials, but from the woody parts of plants that end up as agricultural waste, including straw and sawdust.

What kinds of materials are available depends on the specialisation of the local agriculture. The most promising starting material may be sugar cane residues ('bagasse') in the Caribbean, straw in Canada, and sawdust in Scandinavia. Even food waste, from densely populated areas could be converted into biofuel, as has been demonstrated by the North American Biofuels Company which operates in New York and New Jersey. While the end product, *eg* biodiesel or bioethanol may be indistinguishable from current biofuels, the production pathways will need to be radically different and will require new technology.

Biofuel feedstock - food waste collected in towns and cities could be converted into biofuel © PhotoDisc

The key advantage of the existing, 'first-generation' biofuels is that they are easy to make with established technology, not fundamentally different from that of making vodka or cooking oil. To produce bioethanol, carbohydrates are hydrolysed into sugars that are fermented to form alcohol, which is then distilled. Plant oils from rapeseed or soy beans simply need to be extracted followed by catalytic transesterification to be turned into biodiesel.



Scheme 1 Synthesis of biodiesel

By contrast, making use of the indigestible parts of plants requires complex procedures that can crack their tough structures, which are based on lignocellulose. This fibrous material is made up of cellulose, hemicellulose and lignin. The former two compounds are carbohydrates, which can in principle be hydrolysed into sugars and thus fed into the established procedures to make bioethanol. Separating cellulose and hemicellulose from the unfermentable lignin, however, requires steam and thus a lot of energy. Lignin is currently burnt to generate heat or electricity.

One general approach that can handle the lignin and indeed turn the entire wood into fuel, is the biomass-to-liquid (BTL) process. Fast pyrolysis (heating in the absence of oxygen) of the biomass results in a liquid oil, which can then be refined to syngas (synthesis gas, a mix of carbon monoxide and hydrogen):

$$2C(s) + H_2O(g) \longrightarrow 2CO(g) + H_2(g)$$

thus opening up synthesis routes to a range of products that would normally be made from petroleum.

At the beginning of 2008 Choren Industries in Germany completed building a small industrial refinery for BTL diesel in Freiberg, Saxony, which is expected to run to full capacity by the spring. Shell chemists helped to develop the process used to convert the syngas into diesel fuel, which is a variant of the established Fischer-Tropsch procedure.[1] (The Fischer-Tropsch process, invented by German chemists Franz Fischer and Hans Tropsch in the 1920s, is a catalytic reaction that converts syngas into a range of liquid hydrocarbons similar to petroleum:

$$nCO(g) + 2\,nH_2(g) \longrightarrow (CH_2)_n\,(l) + nH_2O(g)$$

thus allowing the synthetic production of fuels and other petrochemical products. Historically it was used in Germany where coal was abundant and oil scarce.)

The pilot plant is due to produce 13 500 tonnes of BTL diesel per year, using wood waste and straw. In the long term, however, the company has much bigger plans. Choren Industries believes that with wood waste alone, it can produce 2.5 million tonnes of fuel per year, matching the output of 11 traditional petroleum refineries. With this in mind, Choren want to build a large industrial refinery at Schwedt for operation in 2012.

Meanwhile Oxford University spin-out company Oxford Catalysts is also developing new technologies aimed at the production of fuels from wood waste, but is adopting a decentralised approach with a larger number of facilities operating on a much smaller scale. Among other things, the company develops Fischer-Tropsch catalysts that are economically viable in much smaller facilities.[2] The idea is that small, transportable, units could use the waste where it is produced, avoiding the need to transport the biomass which may only hold a small amount of usable energy per weight. With this approach, the large scale flaring of natural gas at oil production sites could be abolished, because gas could be turned into transportable liquids.

At the moment, it still appears possible that radically different approaches may develop into more efficient ways of turning wood and other waste materials into fuels. Chemists in many laboratories around the world are working on improved methods and new catalysts for biomass utilisation. [3] For instance, Ferdi Schueth and his team at the Max Planck Institute for coal research at Mülheim, Germany, have recently shown that a combination of ionic liquids as solvents and solid acids as catalysts can degrade solid wood to small oligosaccharides, which can then be fermented.[4]

New fuels from new biology

While many researchers focus their efforts on recycling agricultural waste and wood, others are looking to produce fuel from scratch. One idea that is rapidly gaining currency is to produce new microorganisms for the industrial production of fuel which will require only carbon dioxide and sunlight for growth. Craig Venter, the geneticist who pioneered the shotgun-sequencing of microbial genomes in the 1990s, and then went on to launch the race for the human genome, is believed to be working on the creation of novel microorganisms which could be tailored towards the production of fuels.

Wouldn't it be good to make use of such waste?© Istockphoto

Part of the appeal is that the metabolic cycles of such organisms could be designed and optimised to the extent that they would produce only desirable products and no waste. However, there will inevitably be ethical concerns over scientists creating new life forms and possible impacts if these escape into the environment.

In a less radical approach, other researchers are considering the advantages of engineering specific biomolecules, particularly enzymes, to degrade lignin. For example, Agrivida,[5] based at Cambridge, Massachusetts, has developed maize plants that produce an enzyme which degrades cellulose. The trick is to make this enzyme switchable so that the plant does not self-destruct while it grows in the field, but can be ordered to degrade its own cellulose after it has been harvested. One promising approach pursued by Agrivida is a temperature switch. By getting the plant to produce a cellulose-degrading enzyme from heat-adapted (thermophilic) organisms, which only becomes active at temperatures around 60ºC, the company can switch on cellulose decomposition simply by heating the biomass to this temperature.

The rapidly growing information on genomes of many different organisms offers other routes towards efficient conversion of biomass to fuels. For instance, the genomes of the microbes degrading cellulose in the stomachs of ruminants could yield as yet unknown enzymes that would help in this endeavour. Moreover, the knowledge of plant genomes could help to identify which plants that are not yet used in agriculture would be best suited for domestication and use as biofuel feedstock. While the traditional domestication of agricultural plants took millennia, the knowledge of modern genomics should enable scientists to derive suitable new varieties within years.

Green fuels from green algae

Another school of thought asks why should we develop new organisms when we have algae? The US Department of Energy (DoE) had funded research into the production of biofuels from algae as part of the Aquatic Species Program from 1978-96, but shifted resources to corn ethanol when it appeared that algal fuels would cost more to exploit. Rising oil prices in 2007-08 have stimulated a renewed interest in the algal alternative.

Algae have the advantage, however, that they don't compete with food crops for land use. They can be grown in purpose built reactors, in ponds created on desert land, and indeed in fenced-in areas of coastal waters. Moreover, much of their biomass will be lipid membrane, which can be transesterified to biodiesel, leaving a residue that will be rich in protein, carbohydrate and water, which can be used as animal feed or fermented to make alcohol.

Green fuels from algal ponds © US DOE/NREL/Gretz, Warren

Solix Biofuels, founded in 2006, is currently developing reactors for the growth of microalgae. The technology may be useful for closed circle recycling of carbon dioxide emissions from power stations. By contrast, PetroSun BioFuels, a subsidiary of the oil company PetroSun, has started growing algae in open saltwater ponds covering 1100 acres in Rio Hondo, Texas. In its purpose-built refinery on site, which was launched in April 2008, PetroSun aims to produce 4.4 million gallons (16.7 million litres) of algal oil per year. Part of the production will be used to make jet fuel.

Other companies, including Chevron and Shell, announced new collaborative projects exploring the possible production of biofuels from algae in 2007 and 2008. Chevron has signed up to a collaboration with the DoE's National Renewable Energy Laboratory (NREL), marking a surprise U-turn for the DoE after 11 years. Shell entered an exploratory project in collaboration with HR Biopetroleum, which already grows algae in ponds on the coast of Hawaii.

In October 2008, the Carbon Trust (UK) announced the 'algae biofuels challenge', a scheme which will pay up to £26 million in grants to develop technology and infrastructures to make algal biofuels viable.

It remains to be seen whether any of these efforts lead to actual fuels appearing at petrol stations. In this field, even the best intentions can be thwarted by unexpected twists and turns of markets and politics. However, with high oil prices and growing awareness of the climate crisis both among politicians and the general public, the time for second-generation biofuels has never been better.

Michael Gross is a science writer based in Oxford. He can be contacted via his website.

References

1. Choren Industries
2. Oxford Catalysts
3. M. Stöcker, *Angew. Chem. Int. Edn*, 2008, **47**, 9200.

4. R. Rinaldi, R. Palkovits and F. Schüth, *Angew. Chem. Int. Edn*, 2008, **47**, 8047.
5. Agrivida
6. E. M. Rubin, *Nature* (*London*), 2008, **454**, 841.

UK's first 'poo bus' goes into service between Bristol and Bath

http://www.bbc.co.uk/news/uk-england-bristol-30115137 20 November 2014

The UK's first bus powered entirely by human and food waste has gone into service between Bristol and Bath.

The 40-seat "Bio-Bus" runs on biomethane gas generated through the treatment of sewage and food waste. The eco-friendly vehicle can travel up to 300km (186 miles) on one tank of gas, which takes the annual waste of about five people to produce. It is run by tour operator Bath Bus Company and will shuttle people between Bristol Airport and Bath city centre. The biomethane gas is generated at Bristol sewage treatment works in Avonmouth, which is run by GENeco, a subsidiary of Wessex Water. GENeco general manager Mohammed Saddiq said: "Gas-powered vehicles have an important role to play in improving air quality in UK cities but the Bio-Bus goes further than that and is actually powered by people living in the local area, including quite possibly those on the bus itself."

- A single passenger's annual food and sewage waste would fuel the Bio-Bus for 37 miles (60km)
- Its combustion engine is similar in design to diesel equivalents in conventional buses
- Compressed gas is stored in dome-like tanks on the roof of the Bio-Bus
- The gas is generated through anaerobic digestion - where oxygen starved bacteria breaks down biodegradable material to produce methane-rich biogas
- To power a vehicle, the biogas undergoes "upgrading", where carbon dioxide is removed and propane added
- Impurities are removed to produce virtually odour free emissions
- Compared to conventional diesel vehicles, up to 30% less carbon dioxide is emitted

The service from the airport to Bath carries about 10,000 passengers each month.Bath Bus Company's Collin Field, said: "With so much attention being directed towards improving air quality generally, the public reaction to the appearance of this bus on a service between a world heritage city and an airport will further focus on the potential for this particular fuel." He said the bus was being launched at a very "appropriate" time, as Bristol is to become the European Green Capital next year.Bristol sewage treatment works processes around 75 million cubic metres of sewage waste and 35,000 tonnes of food waste each year. A total of 17 million cubic metres of biomethane, enough to power 8,300 homes, is generated annually at the plant through a process known as anaerobic digestion.

Batteries:

Batteries for Hybrid and Plug-In Electric Vehicles

http://www.afdc.energy.gov/vehicles/electric_batteries.html

Energy storage systems, usually batteries, are essential for electric drive vehicles, such as hybrid electric vehicles (HEVs), plug-in hybrid electric vehicles (PHEVs), and all-electric vehicles (EVs).

Types of Energy Storage Systems

The following energy storage systems are used in hybrid electric vehicles (HEVs), plug-in hybrid electric vehicles (PHEVs), and all-electric vehicles (EVs).

Lithium-Ion Batteries

Lithium-ion batteries are currently used in most portable consumer electronics such as cell phones and laptops because of their high energy per unit mass relative to other electrical energy storage systems. They also have a high power-to-weight ratio, high energy efficiency, good high-temperature performance, and low self-discharge. Most components of lithium-ion batteries can be recycled. Most of today's plug-in hybrid electric vehicles and all-electric vehicles use lithium-ion batteries, though the exact chemistry often varies from that of consumer electronics batteries. Research and development is ongoing to reduce cost and extend their useful life cycle.

Nickel-Metal Hydride Batteries

Nickel-metal hydride batteries, used routinely in computer and medical equipment, offer reasonable specific energy and specific power capabilities. Nickel-metal hydride batteries have a much longer life cycle than lead-acid batteries and are safe and abuse tolerant. These batteries have been used successfully in all-electric vehicles and are widely used inhybrid electric vehicles. The main challenges with nickel-metal hydride batteries are their high cost, high self-discharge and heat generation at high temperatures, and the need to control hydrogen loss.

Lead-Acid Batteries

Lead-acid batteries can be designed to be high power and are inexpensive, safe, and reliable. However, low specific energy, poor cold-temperature performance, and short calendar and cycle life impede their use. Advanced high-power lead-acid batteries are being developed, but these batteries are only used in commercially-available electric drive vehicles for ancillary loads.

Ultracapacitors

Ultracapacitors store energy in a polarized liquid between an electrode and an electrolyte. Energy storage capacity increases as the liquid's surface area increases. Ultracapacitors can provide vehicles additional power during acceleration and hill climbing and help recover braking energy. They may also be useful as secondary energy-storage devices in electric drive vehicles because they help electrochemical batteries level load power.

Recycling Batteries

Electric drive vehicles are relatively new to the U.S. auto market, so only a small number of them have approached the end of their useful lives. As a result, few post-consumer batteries from electric drive vehicles are available, thus limiting the extent of battery-recycling infrastructure. As electric drive vehicles become increasingly common, the battery-recycling market will likely expand.

Widespread battery recycling would keep hazardous materials from entering the waste stream, both at the end of a battery's useful life, as well as during its production. Work is now under way to develop battery-recycling processes that minimize the life-cycle impacts of using lithium-ion and other kinds of batteries in vehicles. But not all recycling processes are the same:

- **Smelting**: Smelting processes recover basic elements or salts. These processes are operational now on a large scale and can accept multiple kinds of batteries, including lithium-ion and nickel-metal hydride batteries. Smelting takes place at

high temperatures, and organic materials, including the electrolyte and carbon anodes, are burned as fuel or reductant. The valuable metals are recovered and sent to refining so that the product is suitable for any use. The other materials, including lithium, are contained in the slag, which is now used as an additive in concrete.

- **Direct recovery**: At the other extreme, some recycling processes directly recover battery-grade materials. Components are separated by a variety of physical and chemical processes, and all active materials and metals can be recovered. Direct recovery is a low-temperature process with minimal energy requirement.
- **Intermediate processes**: The third type of process is between the two extremes. Such processes may accept multiple kinds of batteries, unlike direct recovery, but recover materials further along the production chain than smelting does.

Separation of different kinds of battery materials is often a stumbling block for the recovery of high-value materials. Therefore, battery design that takes disassembly and recycling in mind is important to the success of PEV sustainability. Standardization of batteries, materials, and cell design would also make recycling easier and more cost-effective.

Battery Swapping

For long-distance travel, where fast charging is not available, battery swapping might be a solution. Tesla Motors is testing battery swap infrastructure that enables drivers to pull into a station and exchange a depleted battery with a fully charged one in less time than it takes to fuel a conventional vehicle. Use of battery swap stations requires a vehicle that has been designed with a swappable battery pack.

Plug-In Hybrid Electric Vehicles

http://www.afdc.energy.gov/vehicles/electric_basics_phev.html

Plug-in hybrid electric vehicles (PHEVs) use batteries to power an electric motor and use another fuel, such as gasoline or diesel, to power an internal combustion engine or other propulsion source. Using electricity from the grid to run the vehicle some or all of the time reduces operating costs and petroleum consumption, relative to conventional vehicles. PHEVs might also produce lower levels of emissions, depending on the electricity source.

Heavy-duty vehicles can be converted to PHEVs and a few light-duty PHEVs are commercially available. Although PHEVs are generally be more expensive than similar conventional and hybrid vehicles, some cost can be recovered through fuel savings, a federal tax credit, or state incentives.

Powered by Electric Motor and Engine

Plug-in hybrid electric vehicles have an internal combustion engine or other propulsion source and an electric motor, which uses energy stored in batteries. PHEVs generally have larger battery packs than hybrid electric vehicles do. This makes it possible to drive moderate distances using just electricity (about 10 to 40-plus miles in current models), commonly referred to as the "all-electric range" of the vehicle.

During urban driving, most of a PHEV's power comes from stored electricity if the battery is charged. For example, a light-duty PHEV driver might drive to and from work on all-electric power, plug in the vehicle to charge it at night, and be ready for another all-electric commute the next day. The internal combustion engine powers the vehicle when the battery is mostly depleted, during rapid acceleration, or when intensive heating or air conditioning is required Some heavy-duty PHEVs work the opposite way, with the internal combustion engine used for driving to and from a job site and electricity used to power the vehicle's equipment or control the cab's climate while at the job site.

Fueling and Driving Options

Plug-in hybrid electric vehicle batteries can be charged by an outside electric power source, by the internal combustion engine, or through regenerative braking. During braking, the electric motor acts as a generator, using the energy to charge the battery. Learn more about charging PHEVs.

PHEV fuel consumption depends on the distance driven between battery charges. For example, if the vehicle is never plugged in to charge, fuel economy will be about the same as a similarly sized hybrid electric vehicle. If the vehicle is driven a shorter distance than its all-electric range and plugged in to charge between trips, it may be possible to use only electric power.

Fuel-Efficient System Design

Beyond battery storage and motor power, there are various ways to combine the power from the electric motor and the engine. The two main configurations are parallel and series. Some PHEVs use transmissions that allow them to operate in either parallel or series configurations, switching between the two based on the drive profile—this is called "blended mode" or "mixed mode."

- **Parallel** hybrid operation connects the engine and the electric motor to the wheels through mechanical coupling. Both the electric motor and the engine can drive the wheels directly.

- **Series** plug-in hybrids use only the electric motor to drive the wheels. The internal combustion engine is used to generate electricity for the motor. General Motors (GM) uses a slightly modified version of this design in the Chevy Volt. GM refers to this design as an extended range electric vehicle (EREV). The electric motor drives the wheels almost all of the time, but the vehicle can switch to work like a parallel hybrid at highway speeds when the battery is depleted.

All-Electric Vehicles

All-electric vehicles (EVs) use a battery to store the electrical energy that powers the motor. EVs are sometimes referred to as battery electric vehicles (BEVs). EV batteries are charged by plugging the vehicle into an electric power source. Although most U.S. electricity production contributes to air pollution, the U.S. Environmental Protection Agency categorizes all-electric vehicles as zero-emission vehicles because they produce no direct exhaust or emissions. Because EVs use no other fuel, widespread use of these vehicles could dramatically reduce petroleum consumption.

Both heavy-duty and light-duty EVs are commercially available. EVs are typically more expensive than similar conventional and hybrid vehicles, some cost can be recovered through fuel savings, a federal tax credit, or state incentives.

Driving Range

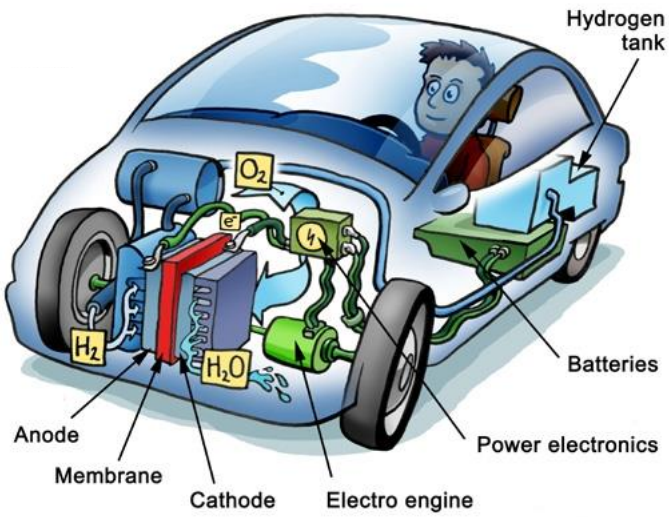
Currently available EVs have a shorter range per charge than most conventional vehicles have per tank of gas. EV manufacturers typically target a range of 100 miles on a fully charged battery. According to the U.S. Department of Transportation Federal Highway Administration, 100 miles is sufficient for more than 90% of all household vehicle trips in the United States. For longer trips, it is necessary to charge the vehicle or swap the battery en route.

The efficiency and driving range of EVs varies substantially based on driving conditions and driving habits. Extreme outside temperatures tend to reduce range, because more energy must be used to heat or cool the cabin. High driving speeds reduce range because of the energy required to overcome increased drag. Compared with gradual acceleration, rapid acceleration reduces range. Hauling heavy loads or driving up significant inclines also reduces range.

Hydrogen Fuel Cells:

http://www.toyota-global.com/innovation/environmental_technology/fuelcell_vehicle/
http://www.ukhfca.co.uk/
Wagner et al's article will be available during the tutorial for use in this and next week's session

Tutorial 2 – Hydrogen Fuel Cells



What is the Purpose of Tutorial 2?

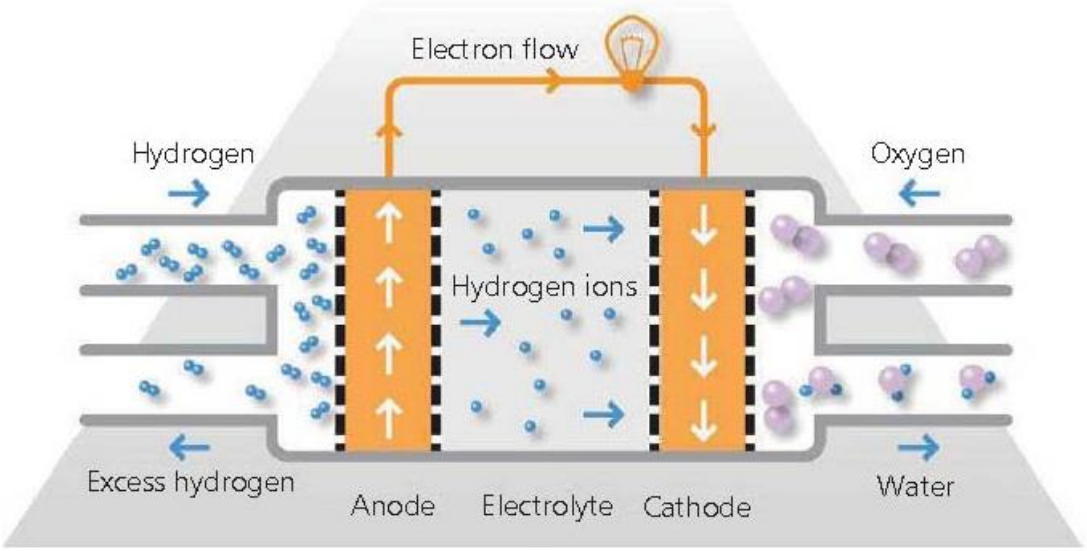
- To understand how fuel cells work.
- To recall oxidation and reduction reactions

Oxidation
Is
Loss of electrons
Reduction
Is
Gain of electrons

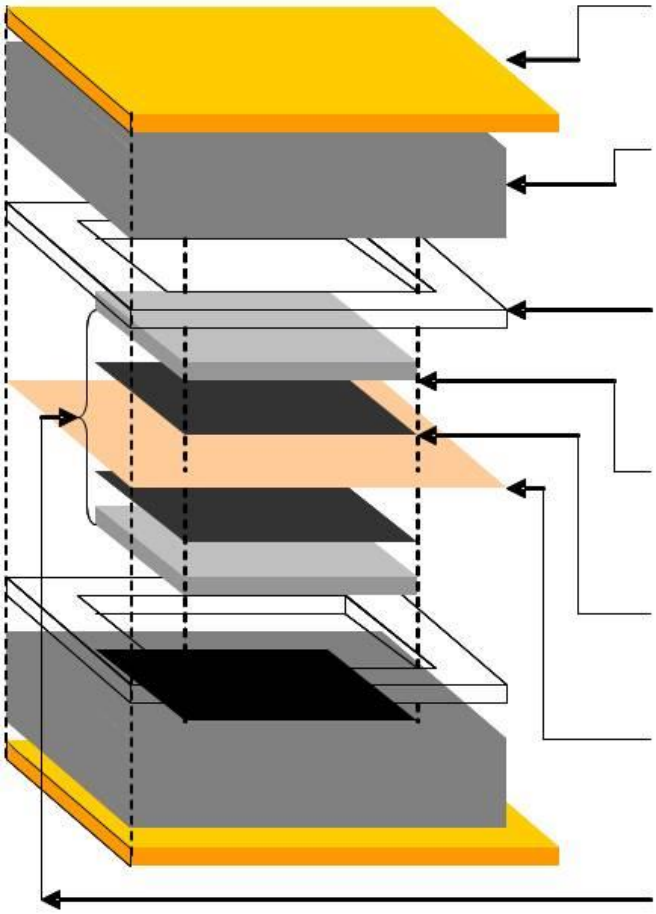
The overall reaction occurring in a Hydrogen Fuel Cell is:

Can you work out the REDOX half equations?
At the anode the Hydrogen is oxidised:

At the cathode the Oxygen is reduced



What goes into a fuel cell stack?



What would happen if the fuel cell components weren't optimised? Think of possible problems for 3 areas of the fuel cell that we've discussed.

Component: Possible Problems: Possible Outcomes	Component: Possible Problems: Possible Outcomes	Component: Possible Problems: Possible Outcomes

Tutorial 2 – Homework

In today's tutorial we have learnt about the components of the Hydrogen Fuel Cells and started to consider their limitations and challenges. This homework will allow you to explore these issues independently and pose probing questions of your own.

Read the Debe article.

Highlight limitations of the fuel cell that the article raises and any concepts you are unsure of.

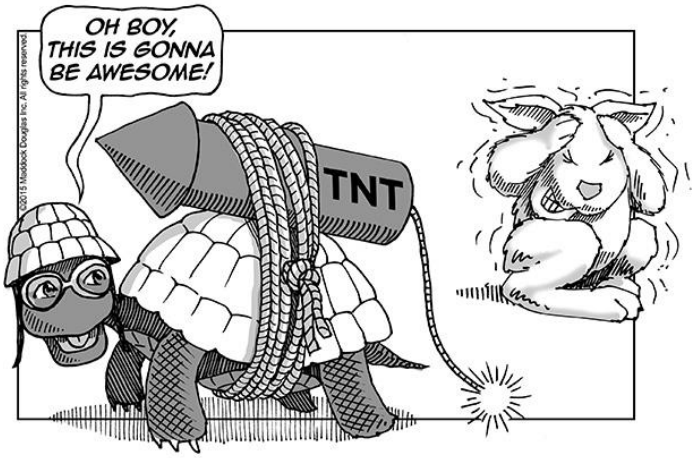
Summarise the limitations of fuel cells in 200-300 words.

Write one question you have after reading the article.

Then try to find a reliable source to answer your question.

You could look at websites hosted by:
-universities
-government agencies (DOE)
-academic journals

Tutorial 3 – Catalysts and their Reactivity



What is the Purpose of Tutorial 3?

- Recap the use of catalysts to increase the rate of reaction
- Why aren't fuel cells 100% efficient?
- To consider current PEMFC catalysts and the factors affecting their reactivity

So why aren't fuel cells 100% efficient?

Look at the potential curve on the left-hand side, the green line represents the theoretical thermodynamic maximum whilst the red line shows the polarisation curves for a state of the art catalyst. What factors could be causing the loss of potential?

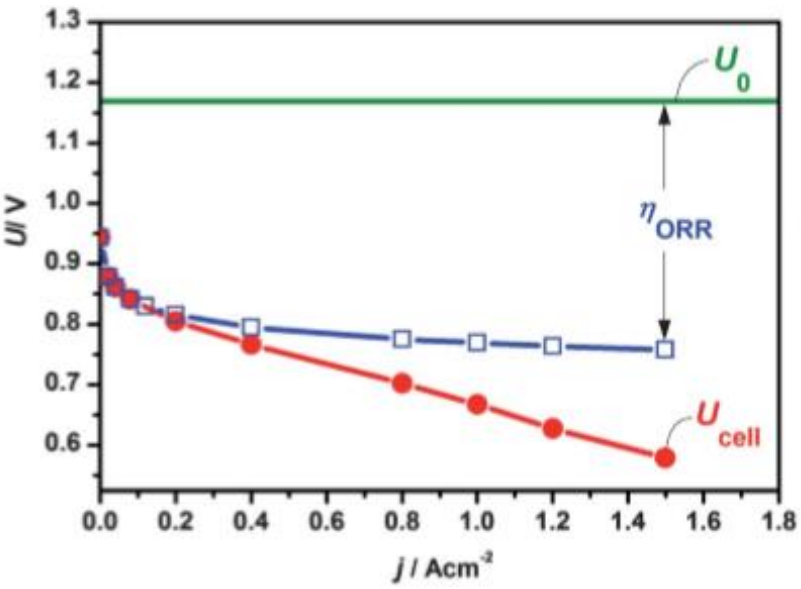


Fig. 1 Polarisation curve of a state-of-the art fuel cell. Operated at 80 °C, at a total pressure of 150 kPa H_2/O_2, adapted from Gasteiger *et al.*[7]

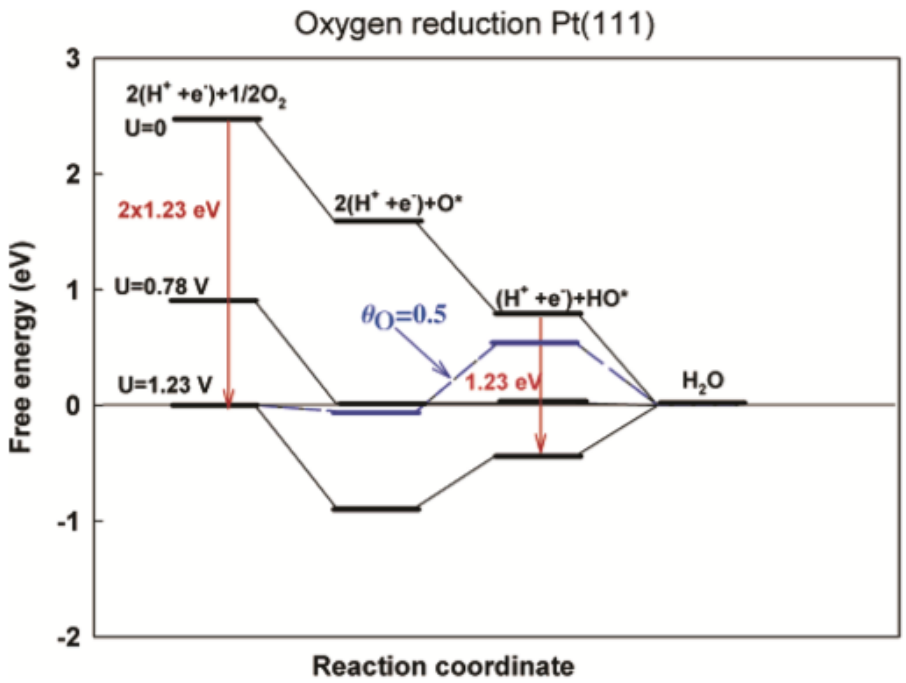
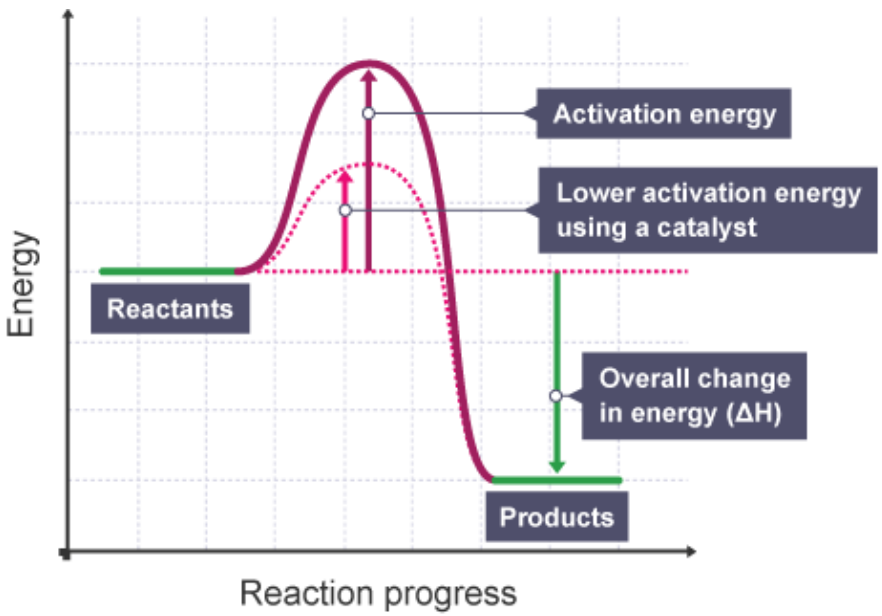
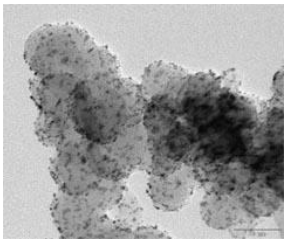


Figure 1. Free-energy diagram for oxygen reduction over Pt(111) based on the energies in Table 1. Results for low oxygen coverage are shown at zero cell potential ($U = 0$), at the equilibrium potential ($U = 1.23$ V), and at the highest potential ($U = 0.78$ V) where all reaction steps are exothermic. For $U = 1.23$ V, the free-energy diagram for the case of an oxygen coverage of $^1/_2$ is included.

The Role of Catalysts



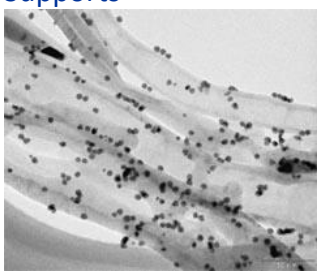
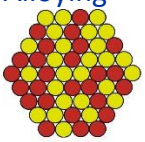
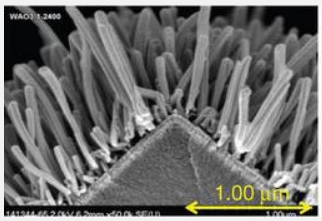
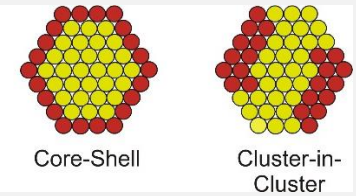
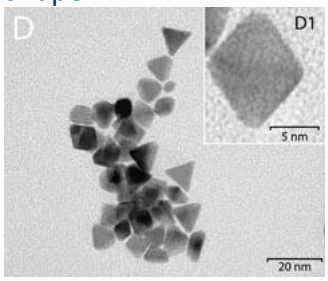
Current Catalysts

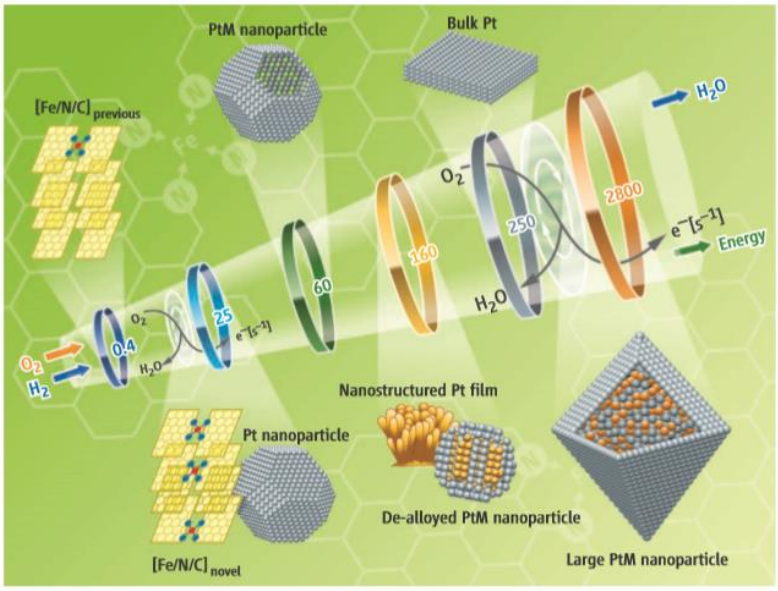


Pt on Carbon black (high surface area C support)

- 5-10nm particles
- Good initial dispersion
- Inexpensive support
- Agglomeration of Pt
- Corrosion of the support

Factors/Solutions

Supports 	Alloying 
Surface Area 	Internal Structure 
Shape 	Other Ideas



Tutorial 3 – Homework

Produce an A3 poster on improving catalyst reactivity. Use the factors affecting reactivity we discussed in the tutorial and conduct further research into how **two** of these have been exploited by scientists. You will have two minutes to present your poster at the start of next weeks' tutorial so make sure you have clear main points. Please ensure that you reference your sources in line with Appendix A

Tutorial 4 – How does Industry develop new Catalysts?

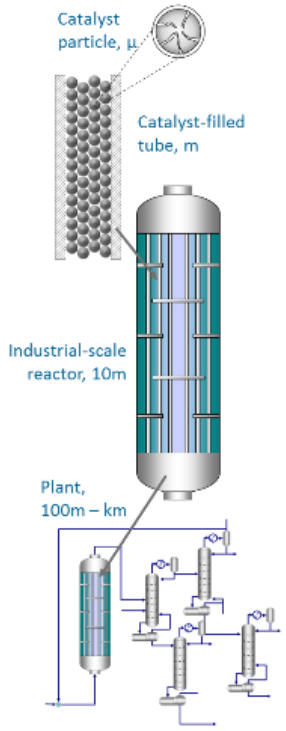
What is the Purpose of Tutorial 4?

- To understand how industrial Research and Development groups in industry work towards new materials.
- To consider the role of different computational techniques in R&D.

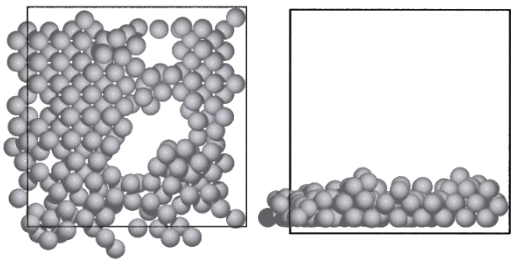
What steps are necessary for Research and Development success?

Computational Methods for R&D applications: Multi-scale challenges

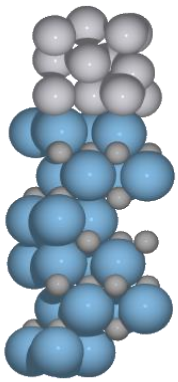
Engineering codes: GPROMS

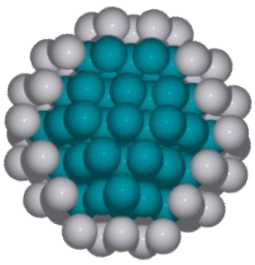


Molecular Mechanics and Molecular Dynamics Simulations



Ab Initio Calculations: Density Functional Theory





Tutorial 4 – Homework: Draft Assignment

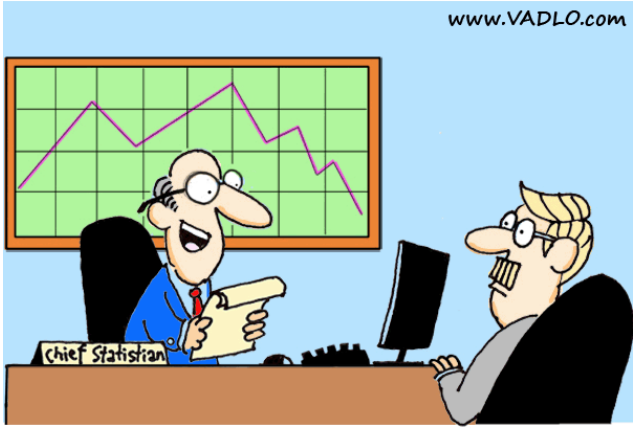
Draw your own R&D flow diagram for the development of an alloyed catalyst. Start by thinking through the research questions that would have to be addressed.

Questions to be addressed:

-
-
-
-

Flow Diagram:

Tutorial 5 – Interpreting Computational Data to make Research Decisions

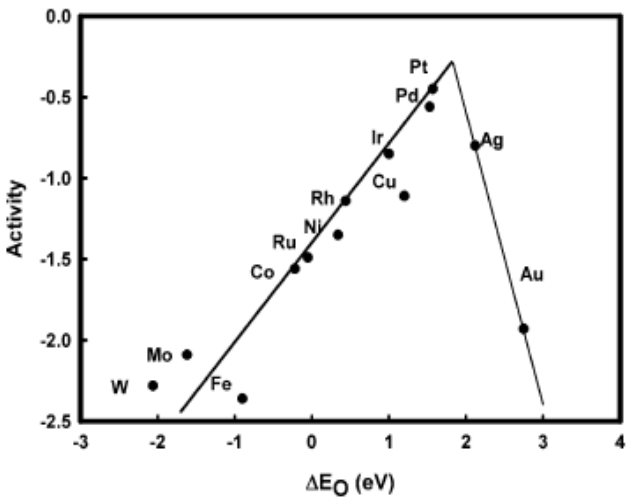


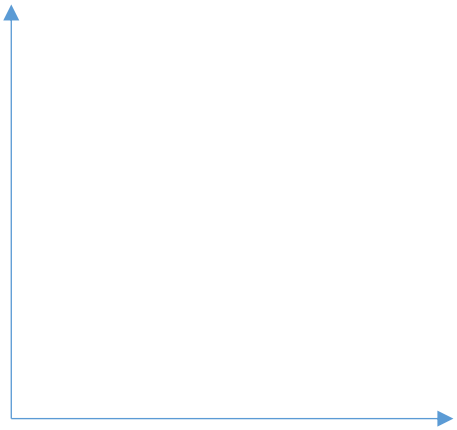
"I can prove it or disprove it! What do you want me to do?"

What is the Purpose of Tutorial 5?

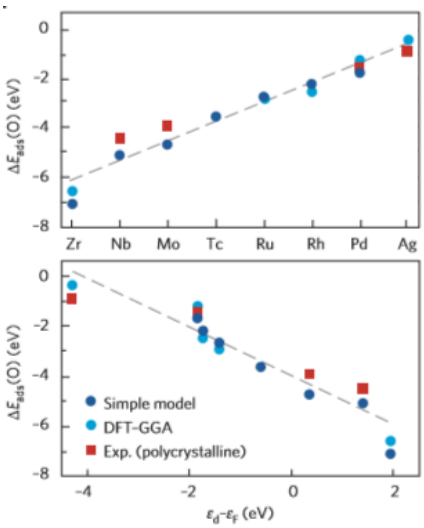
- Introducing the ideas of volcano plots, and descriptors
- Analysis of Data: trends, outliers and limitations
- Introducing the Final Assessment

Volcano Plots and Deciding on Descriptors





What is a Descriptor?



Recapping the Good, the Bad and the Ugly of Data Analysis

Do	Don’t

Tutorial 5 – Homework: Final Assignment

You have been provided with data for 2 novel catalysts being developed for the ORR at the cathode in a hydrogen fuel cell for mobile application.

You represent the R&D department for a large car manufacturer. In view of the Climate Change Act (2008) and other environmental legislation a proof of concept study for hydrogen fuel cells has been commissioned. Write an R&D report concerning the 2 catalysts which have been developed. Assess and evaluate their activity from the data and give recommendations for the further development of one of the prototypes.

Your report should be 2000-2500 words and be appropriately sectioned

Include:

-Your assessment criteria

-Results and Discussion of the provided data

-Recommendations for one of the prototypes to be carried forward and possible routes for further development.

Do read the mark scheme before and after you have completed your report, and make sure to proof read for spelling, grammar and clarity.

Tutorial 6 – Feedback

What is the Purpose of Tutorial 6?

- Reflect on skills learned on the programme with a view to encouraging resilience
- Receive feedback on final assignment

What are the key questions?

- What strengths have I demonstrated in my work and what areas of development are there left for me to address?
- What steps do I need to take to improve my academic output?

Activity 2 – Marking your own

Using the mark scheme, identify three things you did well and three things you could improve.

What went well?

1.

2.

3.

What could be improved?

1.

2.

3.

Activity 3 – Responding to feedback

Read through your feedback sheet and highlight on your assignment where you received positive feedback (one colour) and areas for improvement (different colour). You might find it helpful to annotate this with a brief comment or two.

(Acknowledgement: The structure and the activities in this feedback tutorial were first designed by Hannah Manktelow in January 2015. We have repeated them here as they demonstrate thoughtful and excellent planning, and can be used by all tutors to ensure a successful and productive feedback tutorial.)

Appendix 1 – Referencing correctly

When you get to university, you will need to include references in the assignments that you write, so we would like you to start getting into the habit of referencing in your UniPathways assignment. This is really important, because it will help you to avoid plagiarism. Plagiarism is when you take someone else's work or ideas and pass them off as your own. Whether plagiarism is deliberate or accidental, the consequences can be severe. In order to avoid losing marks in your final assignment, or even failing, you must be careful to reference your sources correctly.

What is a reference?

A reference is just a note in your assignment which says if you have referred to or been influenced by another source such as book, website or article. For example, if you use the internet to research a particular subject, and you want to include a specific piece of information from this website, you will need to reference it.

Why should I reference?

Referencing is important in your work for the following reasons:

- It gives credit to the authors of any sources you have referred to or been influenced by.
- It supports the arguments you make in your assignments.
- It demonstrates the variety of sources you have used.
- It helps to prevent you losing marks, or failing, due to plagiarism.

When should I use a reference?

You should use a reference when you:

- Quote directly from another source.
- Summarise or rephrase another piece of work.
- Include a specific statistic or fact from a source.

How do I reference?

There are a number of different ways of referencing, and these often vary depending on what subject you are studying. The most important to thing is to be consistent. Throughout this project you have been asked to use the Nature 'style', examples of which follow. Referencing includes two elements

A marker in your assignment: After you have used a reference in your assignment (you have read something and included it in your work as a quote, or re-written it your own words) you should mark this is in your text with a superscript number, e.g. i.e. Disney *et al.* reported an increased catalyst activity for their PtRh system.[1] Whilst the use of Rh…..

The next time you use a reference you should use the next number, e.g.[2]

Bibliography: At the end of your work you should include the list of the references you have used in your assignment. In the bibliography, you list your references by the numbers you have used, and include as much information as you have about the reference. The list below gives what should be included for different sources.

The following examples are taken from https://www.citethisforme.com/guides/nature/

For a journal article:

1.Author Surname, Author Initial. Title. *Publication Title* Volume number, Pages Used (Year Published).

Example:

1.Jackson, S. Towards a historical sociology of housework: A materialist feminist analysis. *Women's Studies International Forum* 15, 153-172 (2014).

For a website:

1.Author Surname, Author Initial. Title. (Year Published). at <http://Website URL>

Example:

1.International.gc.ca,. Canada-Korea Free Trade Agreement (CKFTA). (2014). at http://international.gc.ca/trade-agreements-accords-commerciaux/agr-acc/korea-coree/overview-apercu.aspx?lang=eng

For a book:

1.Author Surname, Author Initial. *Title*. Pages Used (Publisher, Year Published).

Example:

1.Tolkein, JRR. The Lord of the Rings, 267-300, (Harper Collins Publishers, 2005)

It would be well worth having a look at Mendeley, which is a free piece of reference managing software. It enables you to import and make notes on articles and resources and cite them in a number of forms (appropriate for different journals!)

Appendix 2- University Applications Guidance

For course choices and careers information:	www.brightknowledge.org.uk
For information and statistics on universities and course:	www.unistats.direct.gov.uk
For comprehensive information on universities, including rankings:	www.thecompleteuniversityguide.co.uk

PLEASE NOTE – The Researchers in Schools programme is designed to support the university applications process at your school. The work you complete for the programme should add to your schoolwork rather than detract from it. Please be aware of deadlines and try to manage your workload appropriately. If you are worried about the programme interfering with your schoolwork then please speak to your teacher.

Subject Specific Top Tips for Strengthening your application

Its well worth doing some research of your own to find out about areas of Chemistry or science in general which you might be interested in for further study- and it'll give your interviewer something to talk about. Find something on the syllabus you were interested by and look for journal articles, books in the library and staff webpages for academics who research that topic. If its Chemistry related the Royal Society of Chemistry website would be a great place to start.

Check out the science lecture series at close by universities- your school should know what's going on- and if you're feeling brave why not email an academic a question about their research to explore a topic further? Then you can show evidence of interest, and progress in your learning.

Make sure if you mention any book or resources in your UCAS application that you actually finish reading them!

Figures

GreenCar Flickr @Doug88888

Tutorial 1

1. Reproduced from IPCC, 2014: Climate Change 2014: Synthesis Report. Contribution of Working Groups I, II and III to the Fifth Assessment Report of the Intergovernmental Panel on Climate Change [Core Writing Team, R.K. Pachauri and L.A. Meyer (eds.)]. IPCC, Geneva, Switzerland, section 1.1, figure 1.1 151p

Tutorial 2

2. Hydrogen Car http://electricvehiclesnews.com/Technology/imagestech/Fuelcell_car_cartoon.jpg accessed 26/10/2015
3. Johnson Matthey Fuel Cells Today Industry Review, 8, (2009)
4. PEMFC schematic from fuelcell.com/fuel-cell-hardware/ accessed 27/10/2015

Tutorial 3

5. Maddock Douglas at http://maddockdouglas.com/sustaining-success-big-companies-need-slow/ accessed 26/10/2015
6. Reproduced from Stephens, I. *et al*, *Energy &Environmental Sci*.,5,5,6744 (2012)
7. Reproduced from Norskov, J. *et al. J. Phys. Chem.B*,108,46,17886-17892,(2004)
8. BBC Bitesize http://www.bbc.co.uk/schools/gcsebitesize/science/triple_aqa/calculating_energy_changes/energy_from_reactions/revision/5/
9.Pt nanoparticles on Vulcan black http://www.leqa.ua.es/en/Research/en-Electrocat1gal.htm
10.Pt on CNT http://www.leqa.ua.es/en/Research/en-Electrocat1gal.htm
11. 3M Pt NSTF catalyst nature.com
12. Pt octahedral nanoparticles http://www.leqa.ua.es/en/Research/en-Electrocat1gal.htm

13&14 Schematic nanoparticle structures http://homepage.usask.ca/~prd822/Research.htm

15. TOF and different catalyst structures reproduced from Gasteiger,H. *Science*, 5923, 48-9, (2009)

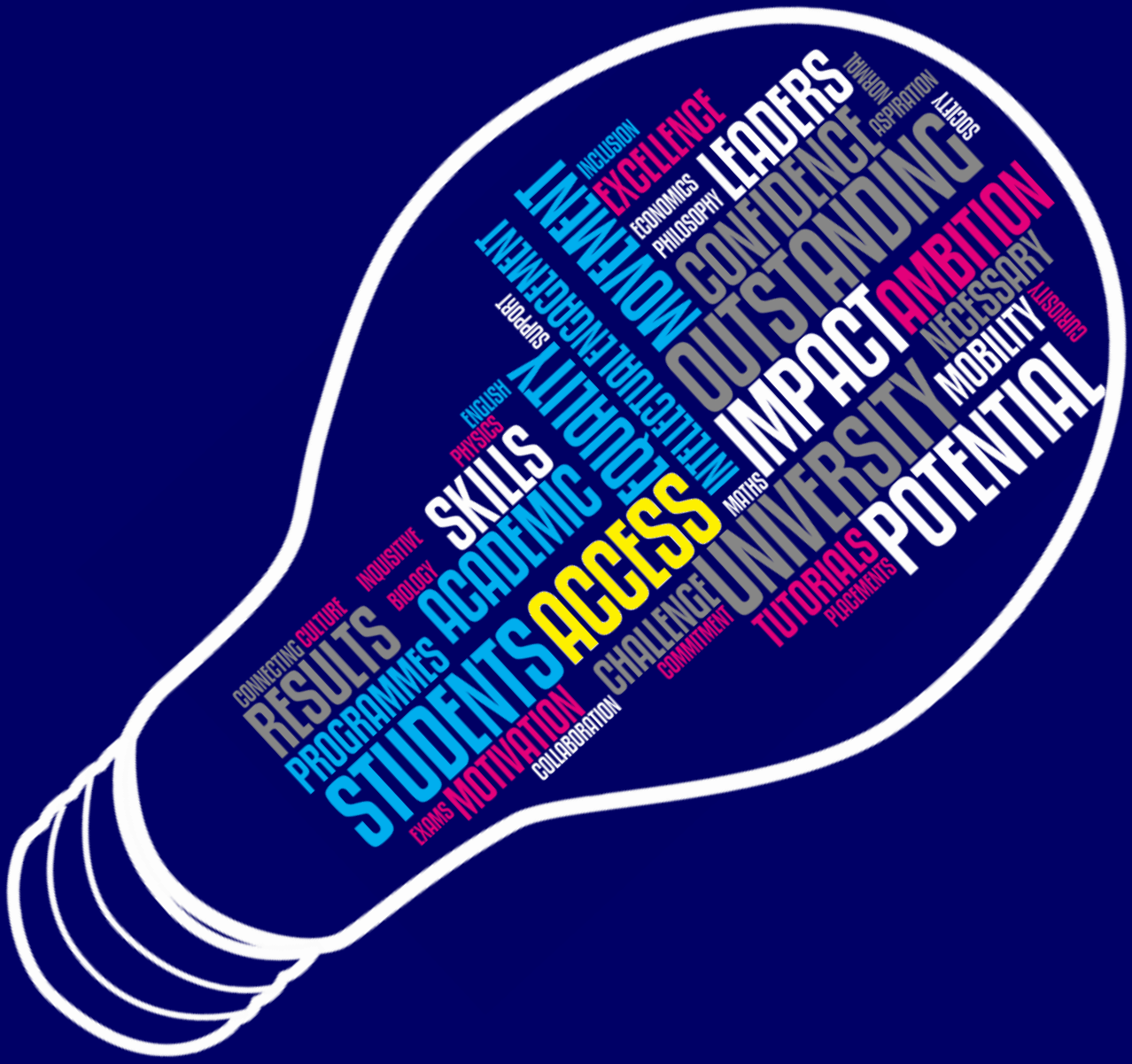
Tutorial 4

16. Catalyst development cartoon Nealo.com
17.GPROMS System http://www.psenterprise.com/concepts/apm.html

18.&19. Author's own images of Pt/carbide systems

Tutorial 5

20.Data cartoon www.vadlo.com
21. Reproduced from Nørskov, J. K. *et al.* Origin of the Overpotential for Oxygen Reduction at a Fuel-Cell Cathode. *J. Phys. Chem. B* **108,** 17886–17892 (2004).
22. Reproduced from Norskov,J. *Nature Chemistry,* 1,1,37-46 (2009)


CONNECTING
CULTURE
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BIOLOGY
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PROGRAMMES
STUDENTS
EXAMS
MOTIVATION
COLLOBORATION
ACADEMIC
SKILLS
PHYSICS
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ACCESS
CHALLENGE
COMMITMENT
EQUALITY
SUPPORT
INTELLECTUAL ENGAGEMENT
MATHS
MOVEMENT
INCLUSION
EXCELLENCE
ECONOMICS
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