Learn Chemistry

Chemistry's Interfaces: The Nano Frontier

Student Guide

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This resource was produced as part of the National HE STEM Programme

National HE STEM Programme

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Registered Charity Number 207890

Table of Contents

The Nano Frontier - Suggested Texts:

Binns C., **Introduction to Nanoscience and Nanotechnology**. Wiley

Atkins P. & de Paula J., **Atkins' Physical Chemistry**. Oxford University Press.

Schmid, G. (editor), **Nanoparticles**, Wiley

Astruc, D. (editor), **Nanoparticles and Catalysis**, Wiley

Ozin, G.A., Arsenault, A.C., Cademartiri, L., **Nanochemistry: A Chemical Approach to Nanomaterials**, RSC Publishing

Daniel, M-C., Astruc, D., **Gold Nanoparticles: Assembly, Supramolecular Chemistry, Quantum-Size Related Properties and Applications toward Biology, Catalysis and Nanotechnology**, *Chem. Rev*., **2004**, 104, 293-346

Session 1 (60-90 minutes)

Pre-Session Preparation

You should be prepared to discuss the following topics in this session:

- Synthesis and stabilisation of gold nanoparticles
- Molecular Orbital Theory and Band Theory in the context of the structure of metals
- Particle in a Box
- Physical and chemical properties of gold nanoparticles
- Surface plasmon resonance
- UV-Visible absorption spectroscopy
- DNA functionalised gold nanoparticles

Intended Learning Outcomes

By the end of this problem you should be able to:

- Describe and compare the different approaches used to synthesise gold nanoparticles and to evaluate these approaches in terms of what is needed to use these nanoparticles
- Describe and compare the mechanisms by which metal nanoparticles may be stabilised
- Explain why DNA functionalisation of the surface of nanoparticles can be used to produce highly selective biosensors
- Explain the origins of the differences in chemical and physical properties of gold nanoparticles with bulk metals as well as individual atoms and molecules (includes an analysis of the electronic structure of transition metal nanoparticles based on molecular orbital, band theory and particle in a box considerations)
- Relate the unique chemical and physical properties of metal nanoparticles to specific applications
- Evaluate the viability of an analytical technique based on a number of factors including sensitivity, reliability, ease of use and cost
- Perform a literature search on an active area of research in order to gain a greater understanding of fundamental scientific concepts are applied to current research
- Work in groups to produce written summaries of scientific research suitable for a range of different audiences
- Prepare for an interview (or in this case a press conference) based on the communication of a scientific concept to a specified audience type (the media in this case)

Facilitation questions

- How big are nanoparticles?
- Why do their physical properties vary from those of the bulk form of the metal or individual atoms or molecules of the metal?
- Why are solutions of gold nanoparticles coloured?
- Why does the colour of solutions of gold nanoparticles vary with size?
- Why does the surface plasmon resonance decrease for nanoparticles with core diameters of around 3 nm and below?
- What other factors can influence the colour of solutions of gold nanoparticles?
- How are DNA functionalised gold nanoparticles commonly used?

World War 2 Era Sub Threatens Northland Communities

A Northland city is facing the lethal legacy of a World War II era submarine which is gradually leaking a toxic metal into coastal waters.

The German U-boat was carrying a cargo of mercury intended for use in weapons production in Japan didn't reach its destination as it was destroyed by allied naval forces off the western coast of Northland in 1945. Although the mercury was never used in the production of weapons, it still poses a serious threat to marine and human life in Northland.

The Northland government has discovered that mercury is slowly leaking from the sunken vessel and is now concerned about sealing up the leak and evaluating the risk to human and marine life from mercury that has already been leaked. The government has decided to seal up the wreckage as it was decided that moving the remains of the boat would possibly result in collapse of the hull leading to a significant increase in the amount of mercury released into the local environment.

"We are very concerned about the impact that this contamination will have both on the local marine population and the inhabitants of the city, we need to act fast to prevent this problem from escalating into a disaster" said Northland's minister for the environment earlier today.

The remains of the U-boat were discovered by the Northland navy earlier this year; it is thought that the broken remains of the boat have been sat on the sea bed off the coast of Northland since at least 1945, possibly leaking mercury the whole time.

The government's Environmental ministry has set up an exclusion zone around the affected area and has banned fishing within a 5 mile radius. The government aims to perform more thorough tests on the levels and distribution of mercury in local waters.

The government is currently investigating a number of techniques that may be used to measure the level of mercury contamination including an experimental technique based on the use of gold nanoparticles. The government will announce more details at a press conference in a week's time.

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From: **Ann Smith [asmith@northland.gov]**

To: **Science team**

Cc:

Subject: **Mercury detection problem**

Dear Team,

As I'm sure you will already be aware, action is being taken to ensure that the no more mercury can escape from the destroyed U-Boat near the west coast of our nation. During routine investigations of mercury levels in coastal waters near Borland, abnormally high levels of the mercuric ion (Hg^{2+}) were detected. We are very concerned that this contamination will affect the local ecosystem and possibly spread into the water sources used by communities near the coast. We have investigated the levels of Hg^{2+} in rivers and streams near the west coast and no contamination has been detected, our fear is that the level of contamination is too low to be detectable by conventional means.

We need to develop a systematic process of testing contamination levels, this process must be cheap to run, portable and accurate at very low concentrations (ca. 1000 pM) of contaminant.

We are considering the use of a new technique to detect this pollution (see reference below). We need you to evaluate the viability of this process compared to existing mercury pollution techniques – remember to pay particular attention to the unique advantages that the new approach offers – a two page summary for circulation to government ministers will suffice. You will also need to write a one page press release informing journalists of what we plan to do which includes information on the background science, you will also need to answer some questions at a press conference.

1. Synthesis of Novel Nanocrystals as Fluorescent Sensors for Hg^{2+} Ions ***Chemistry Letters.***, 2004, **33 (12)** 1608-1609
2. Colorimetric Detection of Mercuric Ion (Hg^{2+}) in Aqueous Media using DNA-Functionalized Gold Nanoparticles ***Angew. Chem. Int. Ed.***, 2007, **46**, 4093 –4096

Yours faithfully,

Ann Smith

The Northland Ministry of Fisheries and Coastal Affairs

Guidance for writing a press release

A good scientific press release should communicate concepts and/or research to a wider audience. Press releases can often lead to wider interest from the press as well as TV & radio journalists

Press releases must be concise, they must have titles with impact (think about how many press releases newspaper editors read – your story must make an impact in the first few words!), and they must get to the point quickly. Press releases most be factual, they need to be timely (i.e. avoid producing press releases on old work and try to produce releases at a time when they will generate interest – see the BBC news story about Olympicene just before the 2012 Olympics as an example!) and they need to be well-written

The opening section should make the following clear:

- Who – did the research?/made the breakthrough?/made the decision?
- What – did they discover?/did they decide?
- When – did they do this?/what was the timescale?/when will it be of general interest?
- Where – was this work done?/will it have an impact?/is it local?
- Why – did they do it?/does this impact on the reader?
- How – was this achieved?

The Press Conference

A press conference is another way of communicating scientific ideas; the press release that you have prepared will form the basis of this conference. A typical press conference will start with a short address from the presenters which summarises the message that they hope to get across. This is followed by a longer period of questioning from the audience (members of the press).

It is important to remember these points:

- This is not a standard oral presentation, the majority of the time you will be answering questions. You should not prepare a PowerPoint presentation!
- Communicate your responses at an appropriate level – the audience won't be experts so it won't be much use to simply quote findings direct from a research paper!
- Critically evaluate your press release and compile a list of possible questions. Put yourselves in the shoes of the press. Some of the things that you may want to think (depending on your decision) about include:
    - Why are you proposing the use of an untested, experimental technique to solve a real-world problem? (i.e. applicable if you have decided to use this new approach)
    - Why are you using older techniques when a new, potentially quicker and more sensitive technique has been described in the research literature? (i.e. if you decide to use another approach to detect the mercury).
    - You may want to think about the timescale and the accuracy of the techniques. Will the chosen technique deliver sufficiently accurate results on a timescale that will protect the local population?

Group reflection (Last 10 minutes of the session)

At the end of this session spend around 5-10 minutes reflecting upon your discussions in this session. You should ask yourselves whether you are confident that you understand the material covered or do you need to carry out further research on some topics?

Construct a brief plan of action – the plan should include a list of the tasks that each group member is expected to do and a timescale for each of these tasks to be done. Remember to include enough time to proof read each other's work before submission. You should briefly present this plan to your tutor before the end of the session.

Session 2

The press conference will take place in this session

Intended Learning Outcomes

By the end of this problem students should be able to:

- Verbally communicate scientific ideas with an audience of peers and to respond to a range of questions on the ideas presented
- Act as ambassadors of science in the community by helping the public gain a deeper understanding of scientific concepts which are often miscommunicated by the media

When you are in the audience, you should engage with the presenting group by asking them questions at a level appropriate for a member of the press. Make sure the presenting group are acting in the best interests in the country (will the safety of local communities by jeopardised, can the nation afford the suggested solution, etc.)

Session 3 (60-90 minutes)

Pre-Session Preparation

You should advise students that they should be prepared to discuss the following topics in the facilitation session:

- The application of functionalised metal nanoparticles as biosensors
- Magnetic nanoparticles
- The use of magnetic nanoparticles in hyperthermic treatments of cancers
- Nanoparticle catalysts
- Surface enhanced effects of metal nanoparticles

Intended Learning Outcomes

By the end of this problem students should be able to:

- Explain the difference in chemical properties of gold nanoparticles in terms of the significantly larger surface to volume ratio of the nanoparticle form of a metal relative to that of the bulk form
- Describe how the unique physical and chemical properties of metal (specifically gold) nanoparticles are (or can potentially be) used in a number of real-world applications
- Perform a literature search on an active area of research in order to gain a greater understanding of fundamental scientific concepts are applied to current research.
- Critically evaluate a number of outline scientific research proposals and rank the proposals based on a number of considerations (e.g. value for money, scientific viability, industrial/social/medical applicability, etc.).
- Write a short report which justifies scientific decisions made (such as the order that the proposals were ranked in).

Northland government announces massive investment in nanoscale science.

Following the recent use of DNA functionalised gold nanoparticles in the detection of mercury pollution levels the government has announced a massive package of investment in nanoscale science. The science minister commented that "this will put Northland at the forefront of this developing area of research. We project that this initiative will promote private investment in Northland and will be yet another contributing factor to the recovery of our economy".

The project was launched with the announcement of government funding for academic research projects which will be distributed by the Northland Physical Sciences Research Council (NPSRC). A research council representative stated "We have an opportunity to develop and support a network of research excellence in the nanosciences. We need to make sure that our academic output encourages the investment of private financial support in this area".

The first research activities to be funded by this project will be announced in the coming weeks.

From: **Science Minister [scienceminister@northland.gov]**

To: **Science team**

Cc:

Subject: **Research council request**

Dear Team,

As part of the recently announced strategic investment programme in fundamental scientific research, we have made a significant sum of money available for projects based on the application of nanoscience to real-world problems. We are very keen to ensure that Northland continues to be a leading force in nanoscale research in Western Europe as we are keen to attract international investment in the commercialisation of this research.

Following your recent research into the use of gold nanoparticles in the detection of mercury contamination, we have recommended that you sit on the research committee panel which will decide how some of the initial funding that we have provided will be allocated. You will be contacted by someone from the committee in due course.

Yours faithfully,

James Smith

Science Minister of Northland

From: **Alan Douglas (Prof) [a.douglas@npsrc.gov]**

To: **Science team**

Cc:

Subject: **Nanoscale projects**

Dear Team,

The government science minister has requested that we include you in the process of allocating funds to innovative nanoscience projects. The first stage of the selection process will be to rank the viability of a number of projects. Please find four outline proposals attached, we need your team to read through each of these and to write a short (approximately 600 word) summary of the science behind each of these outline proposals. It is vital that we select projects which are based on sound scientific concepts and that each project will provide benefits to both the wider scientific community and society. We also need to rank these outline proposals from 1-4 (with 1 being the proposal that you would most like to see funded).

Yours faithfully,

Prof Alan Douglas

Head of the Northland Physical Sciences Research Council

Note - You may assume all of these applications are based on original research and you need not consider financial factors when reviewing these applications.

These outline proposals represent a starting point – you will need to do more research on these topics (you may find the references at the bottom of each outline proposal helpful).

Outline Proposal 1

Dr A. Jenkins, Northland Institute for Sustainable Synthesis and Catalysis

The Development of Novel Gold Nanoparticle Based Catalysts

In spite of the long-held belief that gold is too inert to be used as a catalyst, recent research has shown that gold can behave as a highly active catalyst if it is used in nanoparticle form. The development of novel oxide supported catalysts has been applied to a number of synthetic approaches including the catalytic oxidation of CO by transition metal nanoparticles on oxide supports.[1]

The high surface area to volume ratio of transition metal nanoparticles makes these particles highly accessible for catalytic reaction and therefore increases the reaction activity and the turnover number

We propose the synthesis of a range of gold nanoparticle dendrimers composites which will be tested as catalysts in a number of diverse synthetic processes.

1 S. Galvango and G. Parravano *J. Catal*. **18**, 1978, 320-328.

Outline Proposal 2

Dr B. Paige, Centre for Biological Chemistry, University of Northland

The Use of Functionalised Metal Nanoparticles in the Detection of Biomarkers Associated with Alzheimer's Disease

The use of oligonucleotides-metal nanoparticle conjugates in the detection of specific DNA sequences has developed into a highly active area of research in recent years. The use of metal nanoparticles in the detection of DNA and protein markers for diseases has been motivated by a drive to improve the selectivity and sensitivity of currently used approaches.

The early detection of markers is vitally important in the fight against many diseases. Current detection procedures are often complex, expensive and not portable. The development of simple (and sensitive) nanoparticle based detection methods would remove many barriers to point-of-care treatment which would have a number of benefits on both local and international levels.

The potential improvements in detection sensitivity will allow for significantly earlier detection of specific protein sequences, allowing the diagnosis of conditions (such as cancers) at an earlier stage than possible with current detection approaches, this could potentially have a major impact on the survival rate of many conditions.

Our project will focus on a study of the sensitivity of functionalised metal nanoparticles which can detect ADDL, a potential marker for Alzheimer's disease. This process will followed by monitoring the effect of the antibody concentration on the wavelength maximum of the localised surface plasmon resonance.

Outline Proposal 3

Prof S. Patel, Solid State Physics Department, Netherley University

The Use of Magnetic Nanoparticles in the Treatment of Cancerous Cells by Hyperthermia

Due to the inherent sensitivity of biological cells to small changes in local temperature, cell death can be induced by a heat source. It has recently been demonstrated that magnetic nanoparticles which have been functionalised with an appropriate ligand to specifically bind to cancerous tissue could be used to induce cancer cell death if they are dispersed throughout the target tissue.[1,2] These nanoparticles can be 'activated'

by the application of an external magnetic field which will heat the nanoparticles; this heat is then transferred to the surrounding cancerous cells. If the magnetic field results in a sufficient temperature increase for a sustained period of time, cancer cell death can be induced.

The localised heating of cancerous tissue by magnetic nanoparticles would be a major weapon in the fight against cancer. This project will produce superparamagnetic iron oxide nanoparticles which will be appropriately functionalised for binding to cancerous tissue. The hyperthermic effect of the nanoparticles will be evaluated in ex-vivo conditions to find ensure that the nanoparticles successfully bind to cancerous tissue and to measure how effectively heat is transferred from the nanoparticles to the cells when an alternating magnetic field is activated.

1 Q. A. Pankhurst, J. Connolly, S.K. Jones and J. Dobson*, J. Phys. D: Appl. Phys*. **36**, 2003, R167-R181

2 R. A. Sperling, P. R. Gill, F. Zheng, M. Zanella and W. J. Parak, *Chem. Soc. Rev*. **37**, 2008, 1896-1908.

Outline Proposal 4

Dr J Andrews, Biophysical Group, Department of Physics and Astronomy, Southborough University

The Use of Iron Oxide Nanoparticles in Surface Enhanced Raman Resonance (SERS)

Surface enhanced Raman spectroscopy (SERS) is a powerful and sensitive Raman spectroscopy technique which allows a strongly enhanced signal to be detected from analytes on certain surfaces. The enhancement of Raman signals can be described by either Physical or Chemical mechanisms. This technique will be used to identify the genes sequences in a number of different viruses including HIV and the Hepatitis virus.

Facilitation Questions

Catalysis

- Why are gold based catalysts of limited use to chemists?
- Why do the catalytic properties of gold nanoparticles vary so greatly to those of the bulk form of gold?
- What are dendrimers? How are they used to functionalise nanoparticles?

Biochemical applications

- What are oligonucleotides and how do they relate to DNA?
- What is meant by the term ‘selectivity’ in the context of biosensors and why are these functionalised nanoparticles so selective? Would these biosensors work if the same DNA sequences were applied in the absence of the metal nanoparticle? If not, why not?
- What approaches can be used to functionalise gold nanoparticles with DNA sequences?

Nanomedicine

- What is meant by the term ‘hyperthermia therapy’? How is this effect achieved in this research?
- What makes certain nanoparticles magnetic?
- What is paramagnetism? How is superparamagnetism different?
- Apart from their magnetic properties, what else makes nanoparticles particularly suitable for this application?

Surface Enhanced Raman Sensing

- What is Raman spectroscopy?
- What is Surface Enhanced Raman Scattering?
- How do metal nanoparticles enhance the Raman signal?

Group reflection (Last 10 minutes of the session)

- At the end of this session spend around 5-10 minutes reflecting upon your discussions in this session. You should ask yourselves whether you are confident that you understand the material covered or do you need to carry out further research on some topics?
- Construct a brief plan of action – the plan should include a list of the tasks that each group member is expected to do and a timescale for each of these tasks to be done. Remember to include enough time to proof read each other's work before submission. You should briefly present this plan to your tutor before the end of the session.

Session 4 (60-90 minutes)

Intended Learning Outcomes

By the end of this problem you should be able to:

- Give a short scientific presentation to a varied audience justifying a decision to back a research project.
- Justify a decision to back a given scientific project by considering the relative merits (including value for money, scientific viability, industrial/social/medical applicability, etc.) of a number of alternative courses of action.
- Demonstrate a clear understanding of the background science of a chosen area of scientific research
- Describe similar work that has been done by other groups in a chosen same research area
- Critically evaluate scientific presentation given by other groups and ask questions based on the viability of the decision presented by those groups.

From: **Alan Douglas (Prof) [a.douglas@npsrc.gov]**

To: **Science team**

Cc:

Subject: **RE: Nanoscale projects**

Dear Team,

Thank you for submitting your reports and your rankings. We would like to invite you to present your decision at a short seminar for government ministers (with a range of backgrounds). You will be given 15 minutes (including questions) to present your chosen proposal.

Best wishes,

Prof Alan Douglas

Head of the Northland Physical Sciences Research Council

Aim of this session:

Give a short oral presentation (around 10 minutes long followed by up to 5 minutes of questions from the audience) on your decision. Your presentation must make it clear what your preferred proposal is and must justify this in terms of the background science. You will be expected to ask questions to the other groups at the end of their presentations in order to