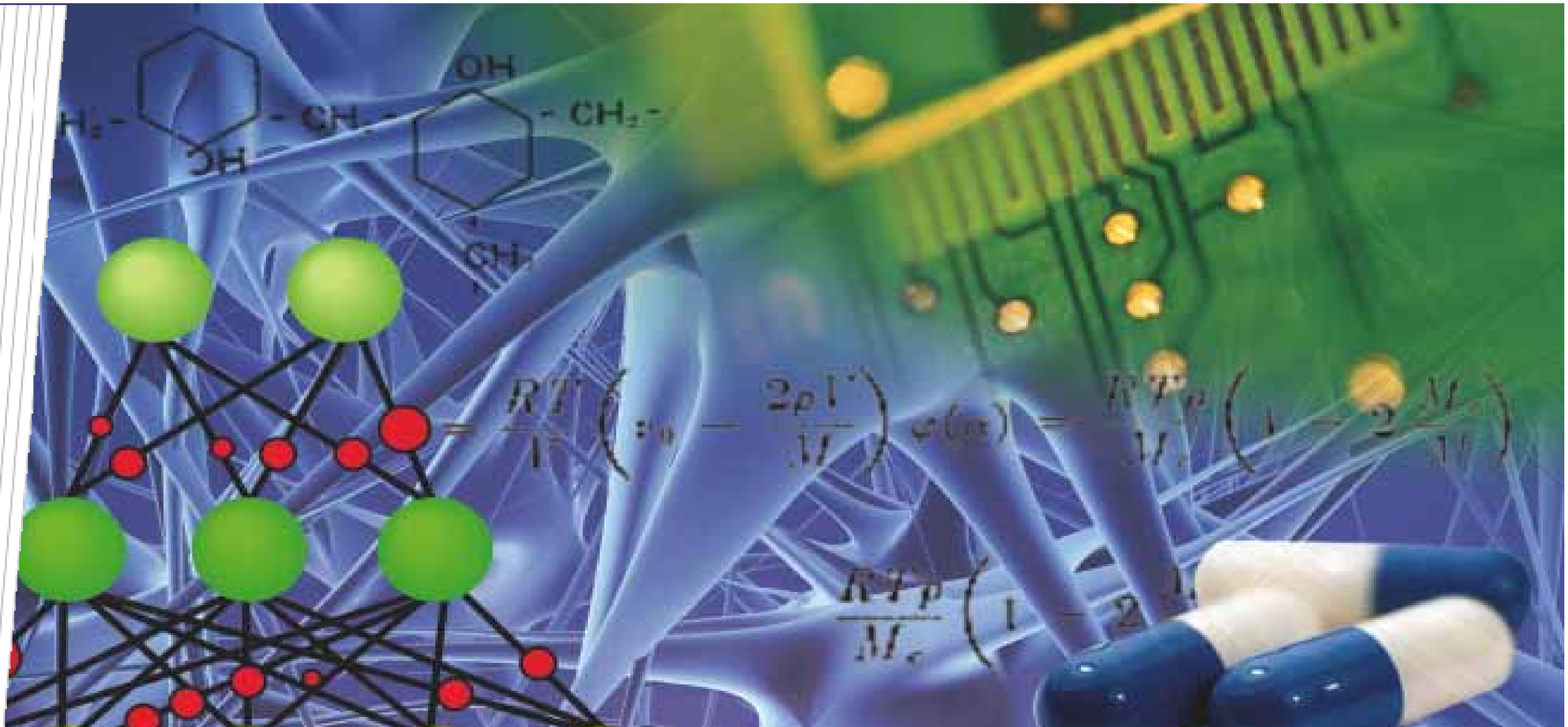


www.csiro.au

Advanced Materials Transformational Capability Platform

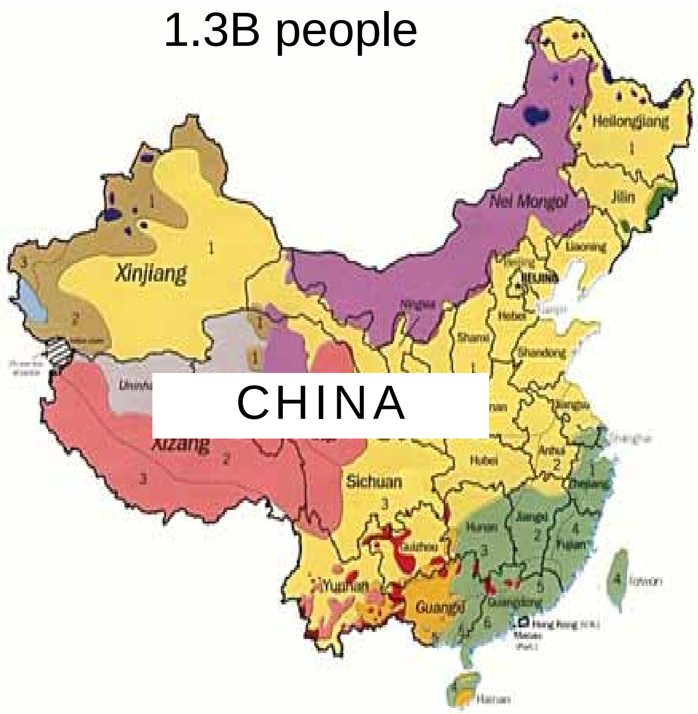
We will use any thing to solve big problems

Dr Cathy Foley
Advanced Materials TCP Coordinator

CSIRO

Australia Not Austria

1.3B people



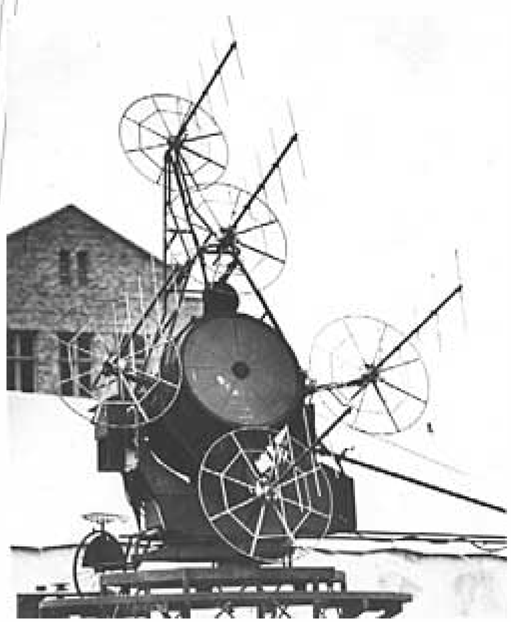
.02B people

EQUATOR

Shanghai has the same population as the whole of Australia

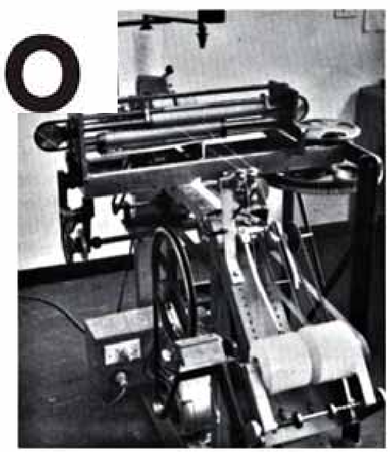
Unique

Began in 1926



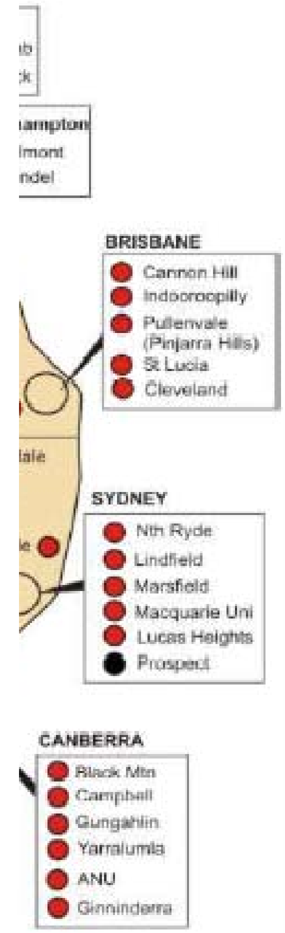
CSIRO

Good science
Solving big Australian
problems



CSIRO

- **Research and development in fields of economic, social and environmental importance:**
  - Agriculture
  - Environment
  - Information and communication technologies
  - Health
  - Advanced materials and manufacturing
  - Minerals and energy
  - Services
  - Transport and infrastructure



CSIRO LOCATIONS

Materials Research CSIRO

- **2007 audit of Materials Research in CSIRO**
  - About 640 materials researchers across CSIRO
  - <3% using combinatorial and high throughput approaches
  - <8% using theory and simulation
  - Majority of work was using traditional materials research approaches with standard and aging infrastructure and equipment

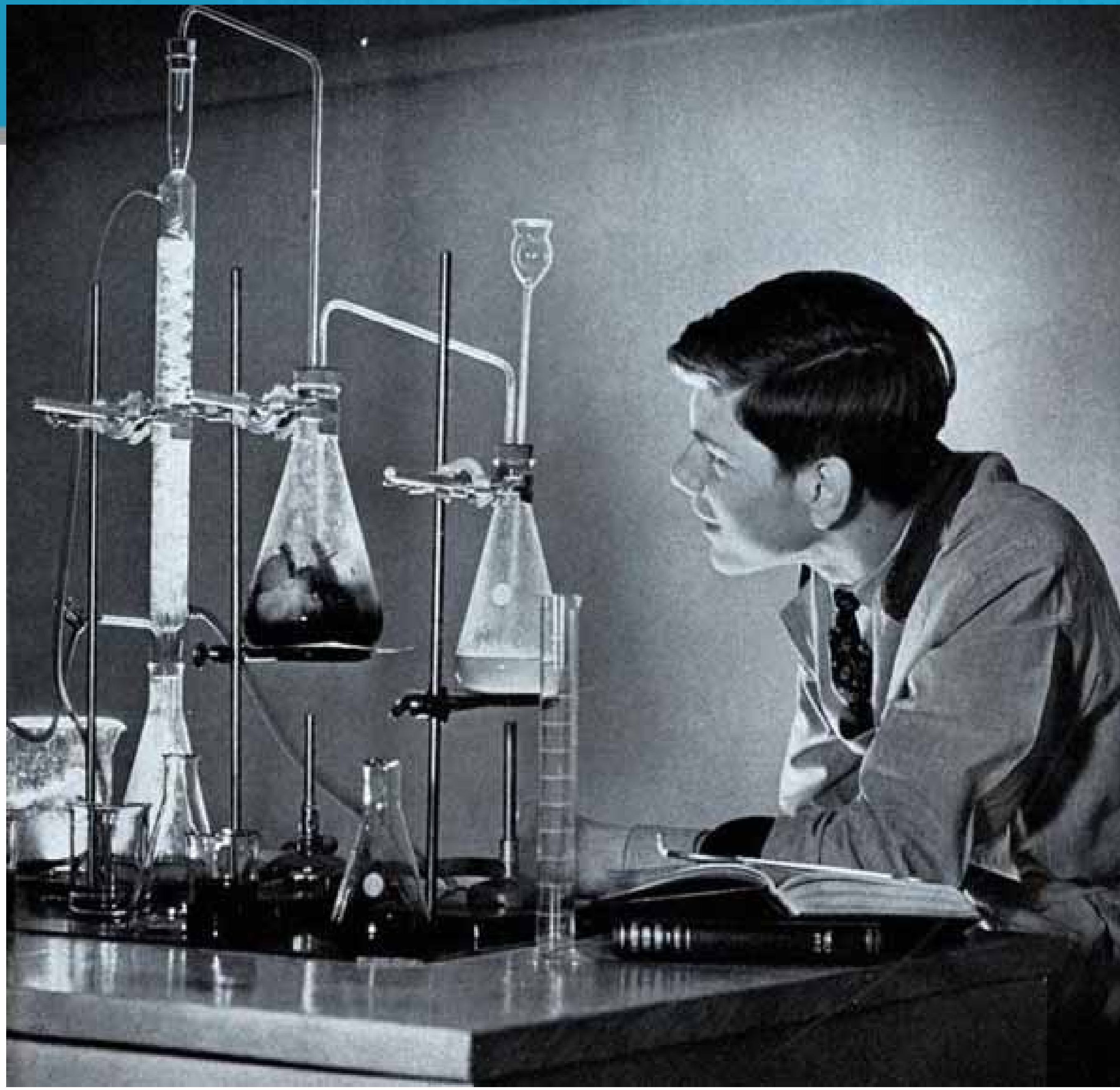
Major Challenges

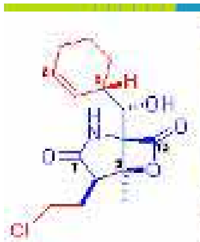
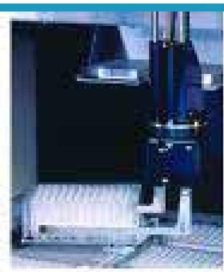
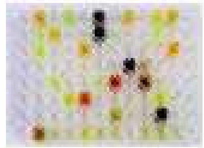
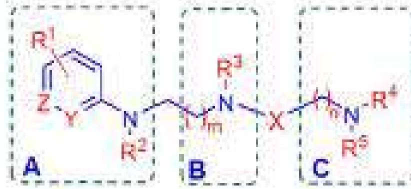
- Climate change
- Energy
- Water
- Sustainable manufacturing
- Aging
- Health
- Food supply
- Globalization
- Transport
- Telecommunications
- Population

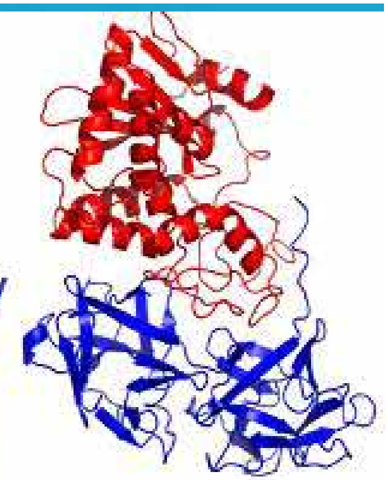
Advanced Materials Transformational Capability Platform

- Disruptive change
- Materials with
  - **Extreme properties**
  - **Disparate properties**

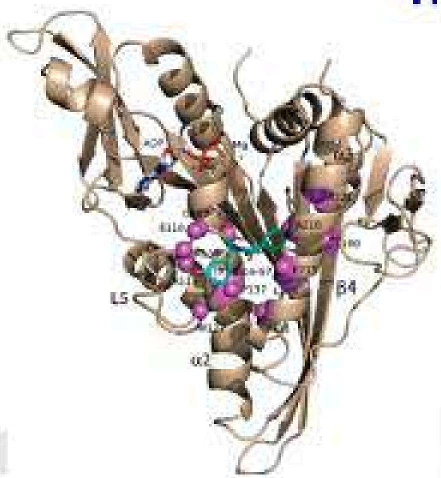
- What we are doing
  - **Large asset investment**
  - **New concept materials characterisation**
  - **Exemplar projects**
  - **Nanosafety**
  - **Networking and training**

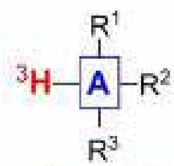
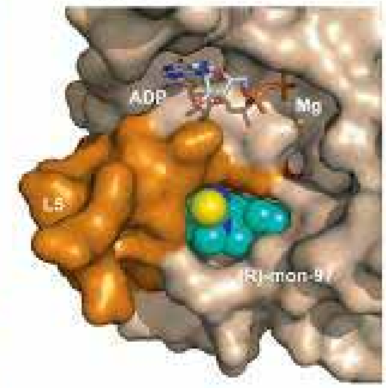


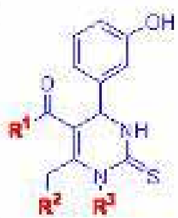







High Throughput Screening & Combinatorial Chemistry



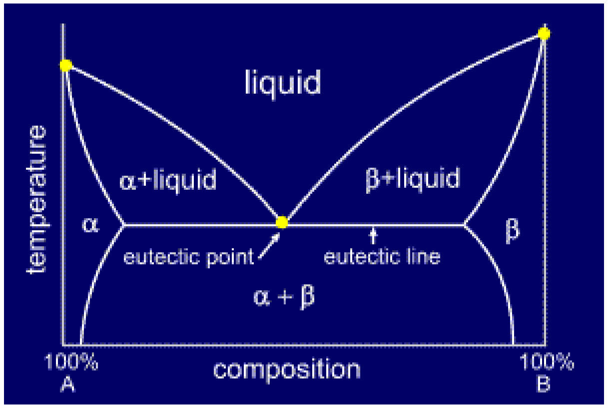







What is different about advanced materials research compared to ordinary materials research?

The tried and true way of materials development



"One graduate student, one alloy, one PhD"*

i.e. it was taking 3 years to develop a new phase diagram

*With apologies to Prof Andrew Murray of Harvard Uni

This talk

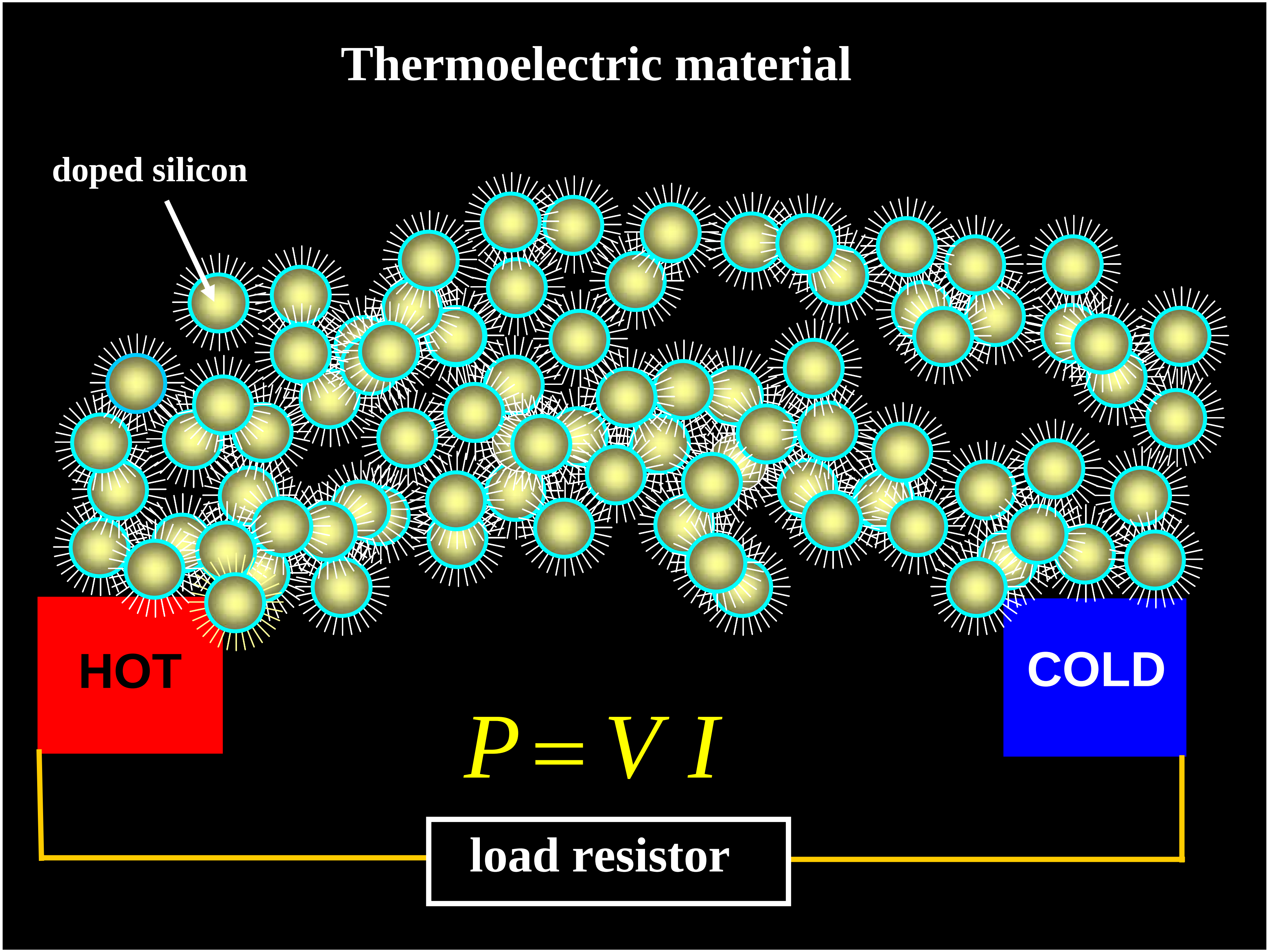
- **What is CSIRO?**
- **Advanced Materials Transformational Capability Platform**
- **Modelling and theory: materials by design**
- **High Throughput and combinatorial materials development: optimizing materials quickly**
- **Bio-inspired materials**
- **Materials informatics**
- **Safety**
- **Conclusions**

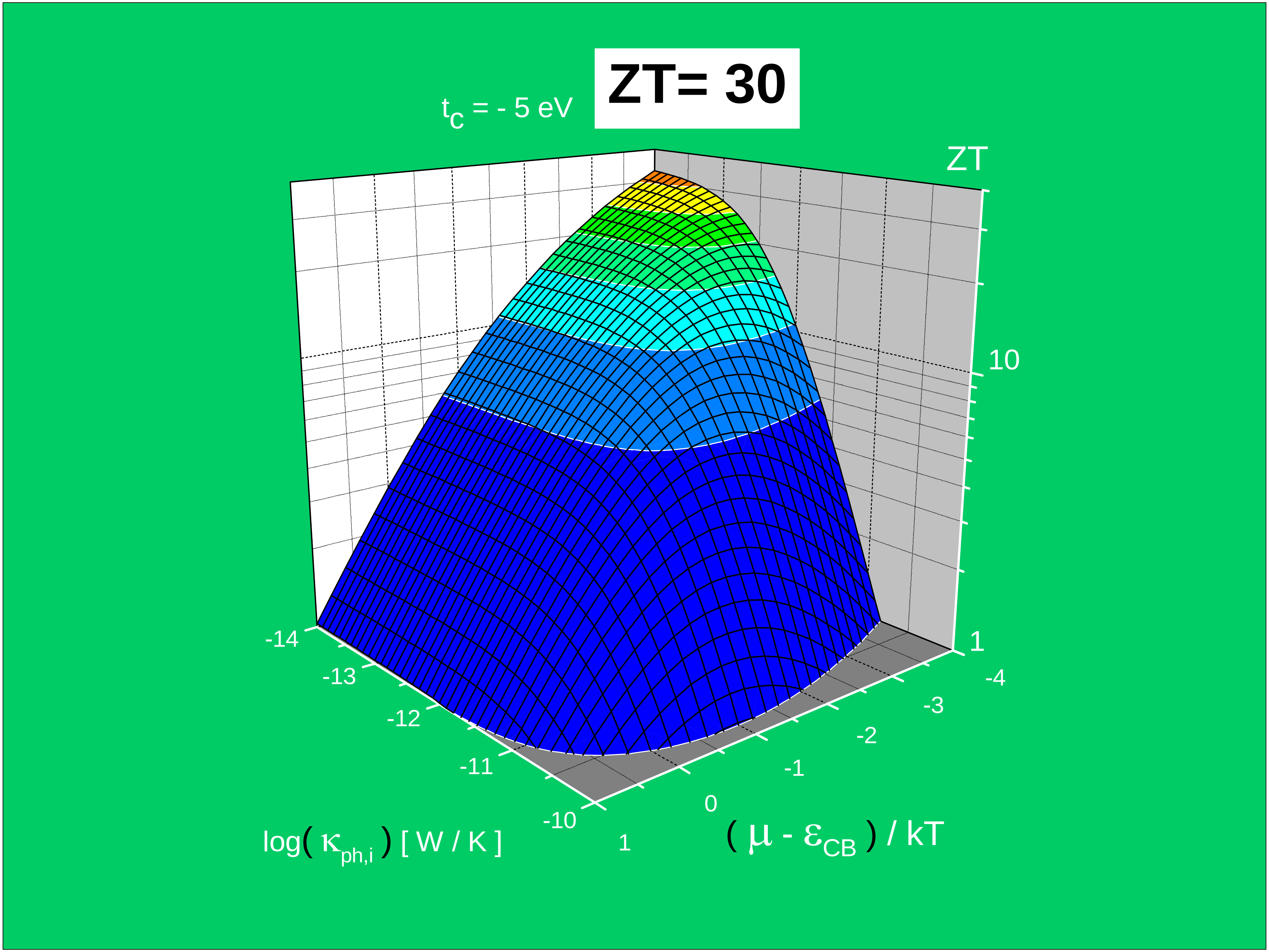
Exemplar Projects

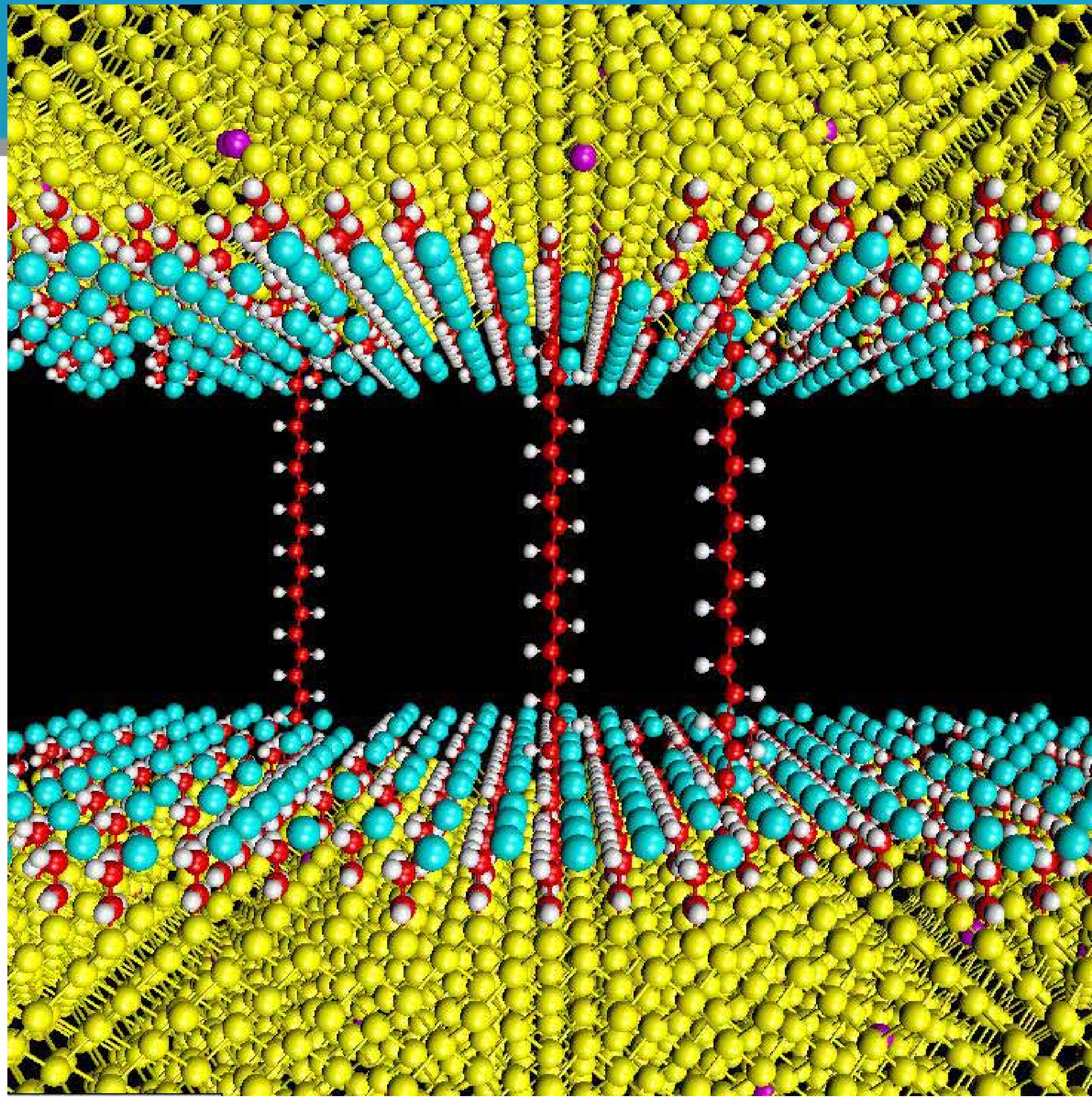
- **High Throughput and Combinatorial Materials development**
  - Organic
  - Inorganic
  - Metal-organic
- **Theoretical and simulation methods of materials design**
  - New concept
  - Hybrid
  - Revolutionary materials design
  - Virtual experiments
- **Highly speculative new materials**
  - Extremely disruptive if successful

Theory and Modelling

- **Design new materials**
- **Predict behaviour and properties**
- **Virtual experiments**

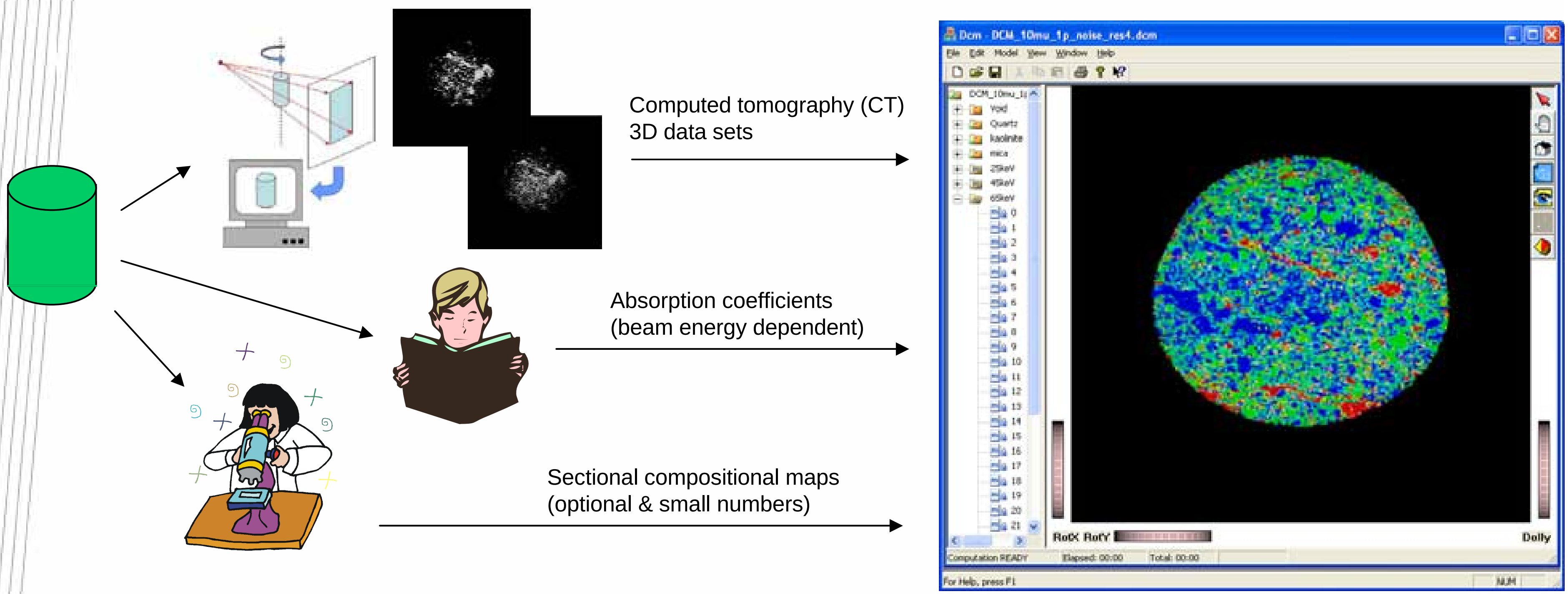

Thermoelectric material
doped silicon
HOT
COLD
P = V I
load resistor


ZT= 30
t_c = - 5 eV
ZT
10
1
-14
-13
-12
-11
-10
1
0
-1
-2
-3
-4
log($\kappa_{ph,i}$) [W / K]
(μ - ε_{CB}) / kT



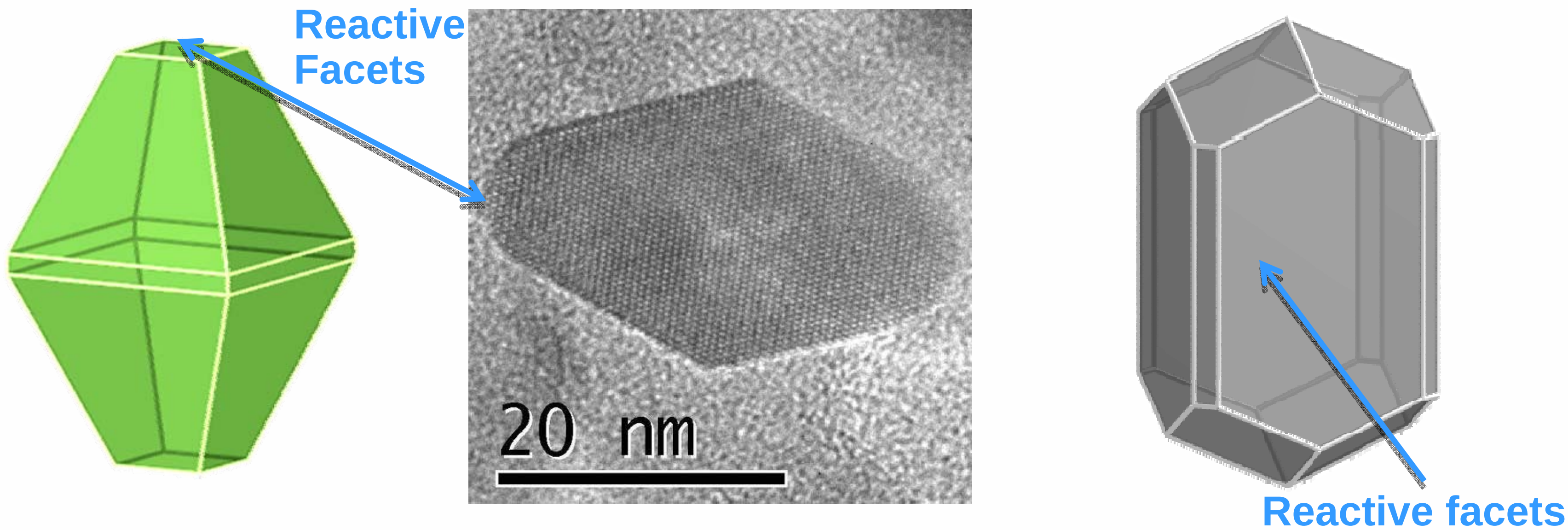
Virtual Experiments

- Combined real conventional CT data with virtual monochrome synchrotron x-ray CT
- Use of true colour for real materials instead of pseudo colour for approximate representations
- Use DCM software tools developed under CSS TCP
- Feasibility study of characterisation of hydrocarbon reservoir shale rock microstructures and properties



Predicting Nanomorphology of TiO_2

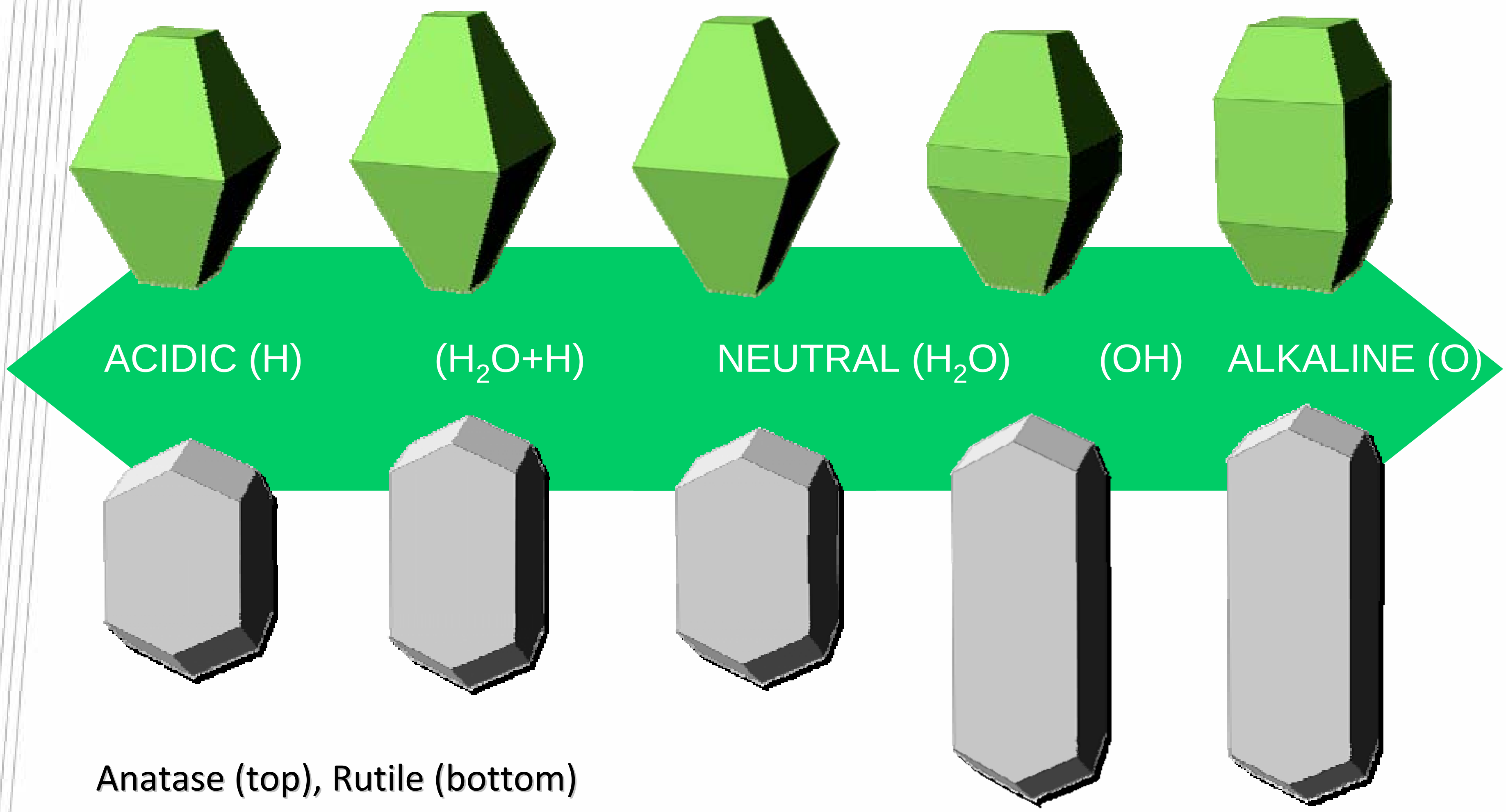
- **Calculate thermodynamic properties using accurate ab initio high performance computer simulations**
  - Insert them into the multi-scale shape-dependent model to predict the most probable shapes of *x* = Anatase and Rutile … for any size



- **Predicted shape for 20 nm Anatase (left), Transmission Electron-micrograph of real 20 nm Anatase nanoparticle (centre), and predicted shape of 20 nm Rutile nanoparticle (right) … in UHV**

A.S. Barnard and P. Zapol, *Phys. Rev. B* (2005)

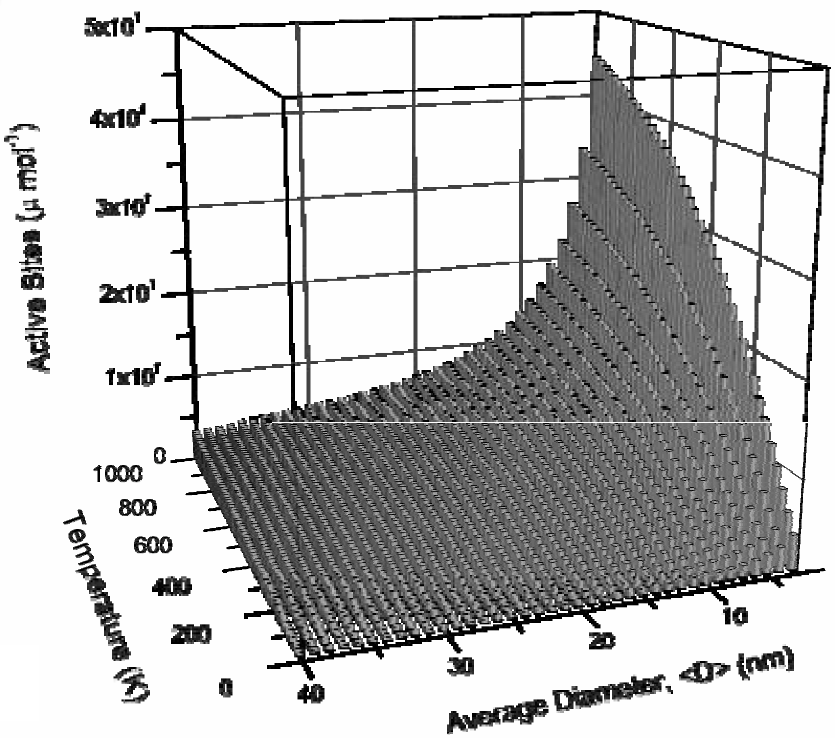
Shape and Surface Chemistry



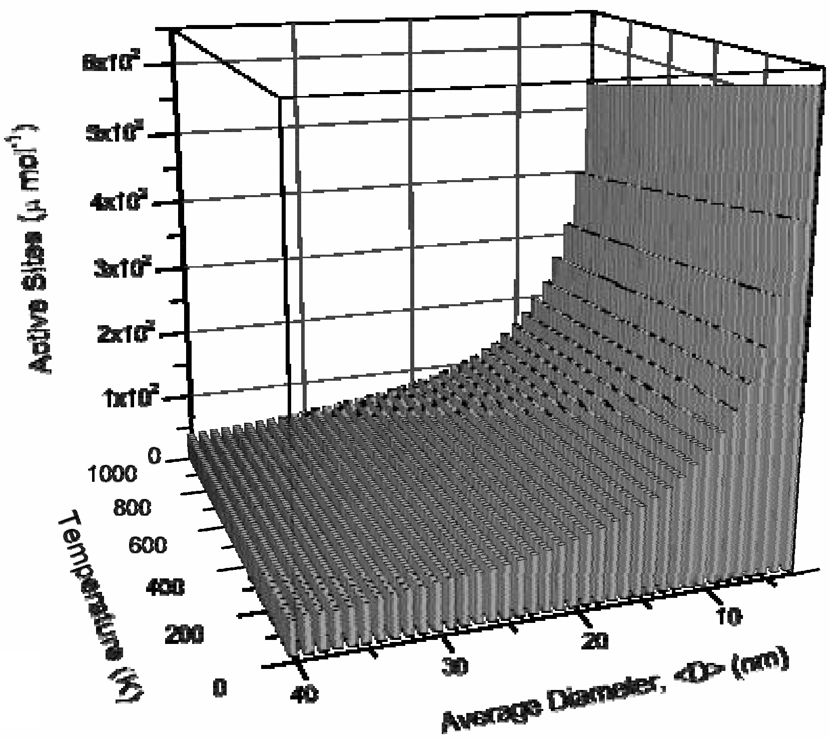
Anatase (top), Rutile (bottom)

A.S. Barnard and L. A. Curtiss, *Nano. Lett.* (2005)

Environmental Impact:
What can TiO_2 do to the environment?



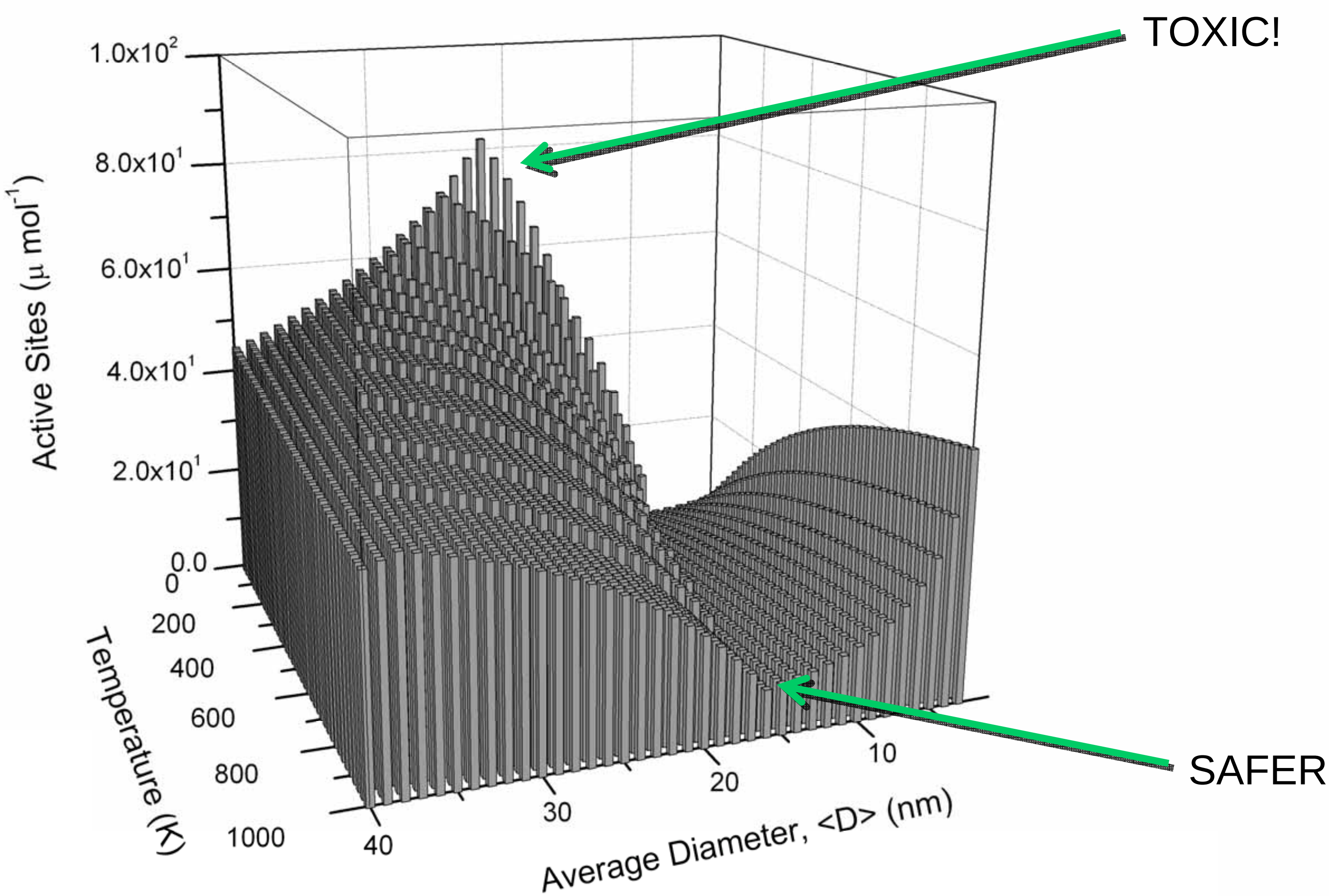
H_2O-terminated ANATASE
(Thermodynamically Preferred)



OH-terminated RUTILE
(Thermodynamically Preferred)

A.S. Barnard, *Nature Nanotech.* (2009)

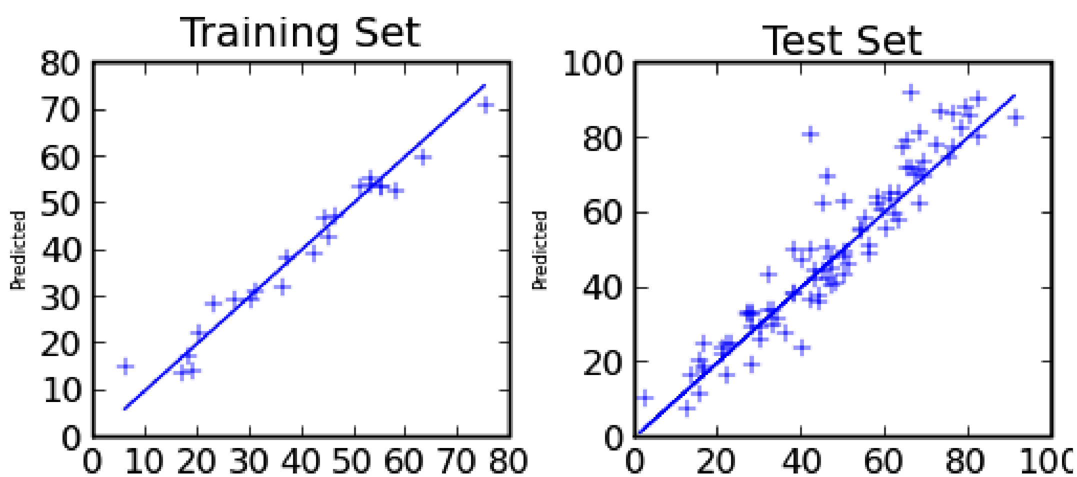
Mapping Potential Ecotoxicity

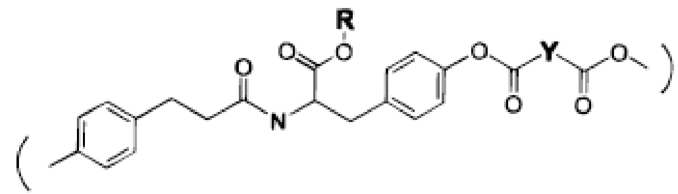


A.S. Barnard, *submitted for publication* (2009)

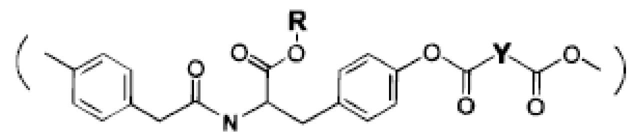
Quantitative **S**tructure-**P**roperty **R**elationships modelling of materials

- Aims to develop and validate platform methods for predictive modelling of diverse materials properties.





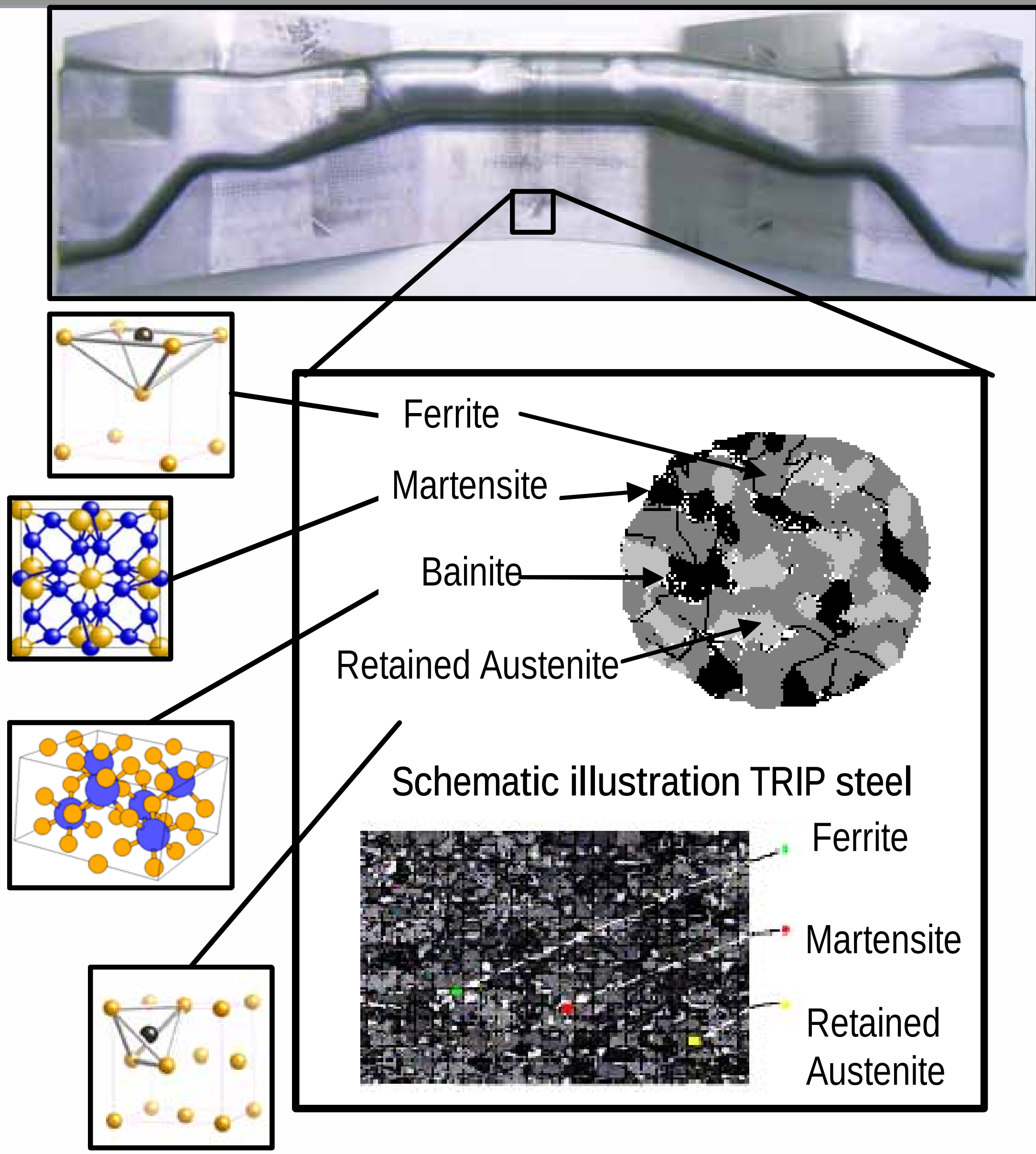
1a



1b

QSPR modelling of Tg of library of 112 polymers.
Model developed using 17 polymers (left) accurately predicted Tg of 95 polymers (right)

MultiScale Modelling

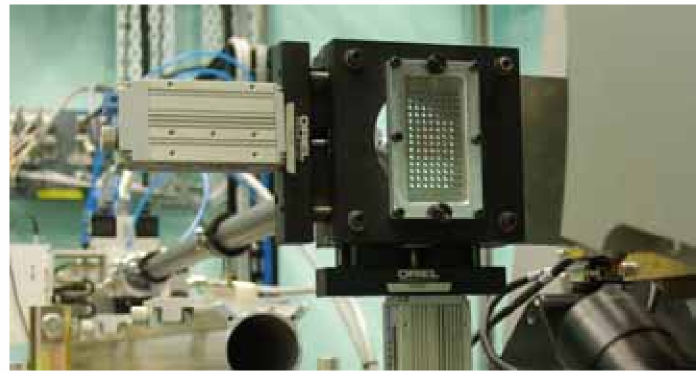


High throughput and combinatorial methods

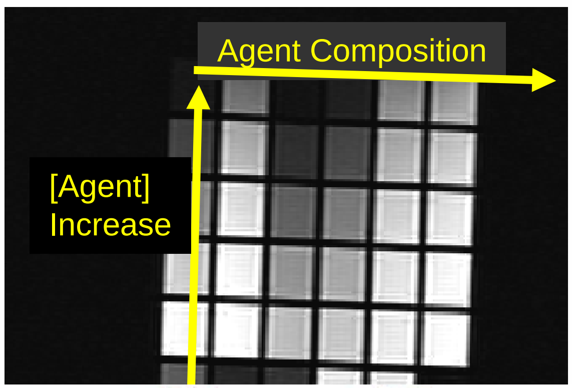
Development of Capability for High Throughput Metal-Organic Frameworks

HT Synthesis

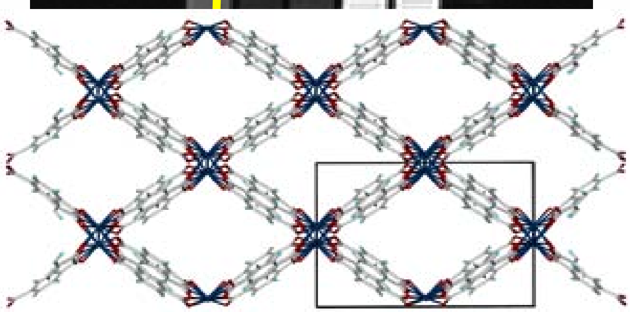
HT Characterisation



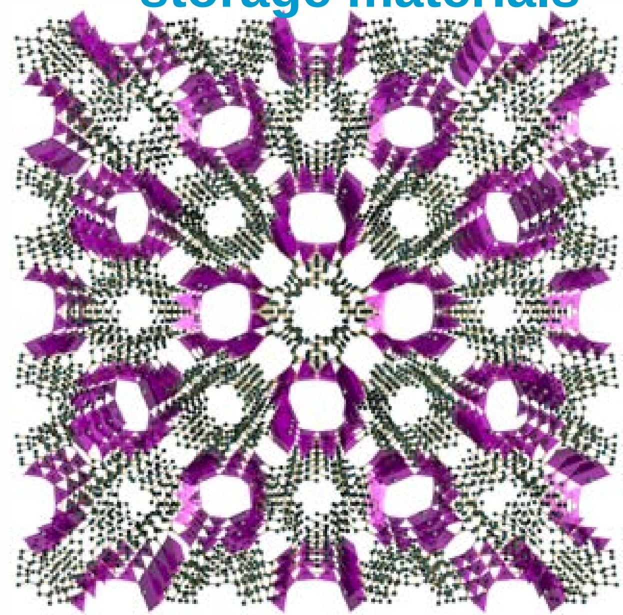
HT Screening



MOFs as MRI contrast agents

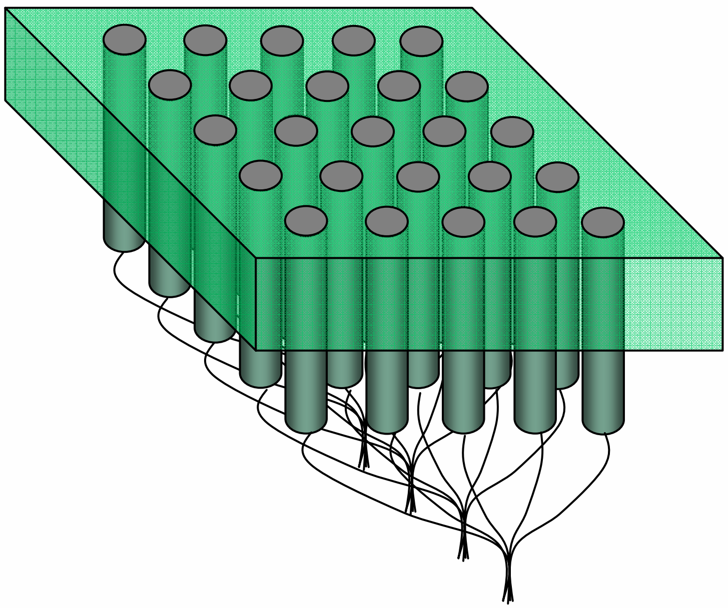


MOFs as hydrogen storage materials

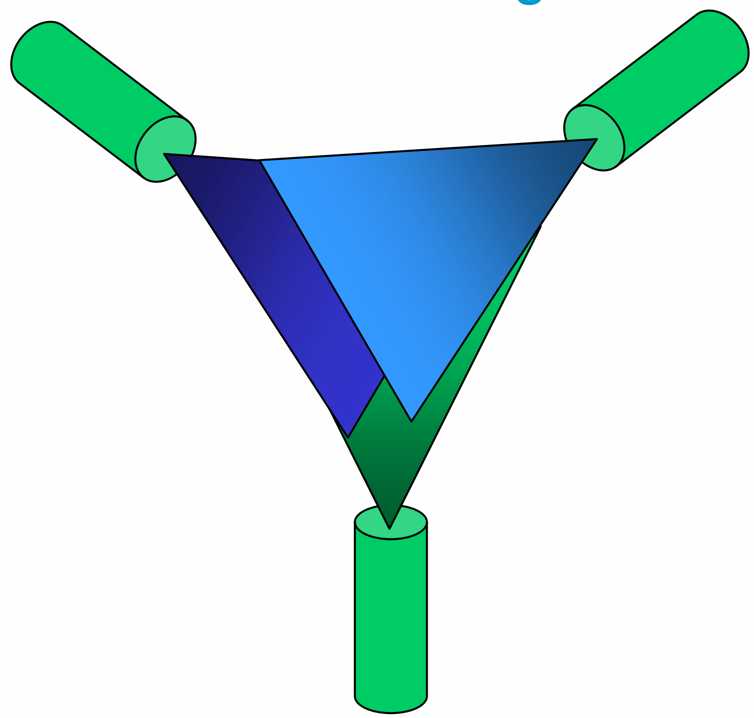


High Throughput Inorganic Coatings

- **Combine multielectrode electrochemical analysis with the deposition of combinatorial libraries of inorganic coatings.**



Multielectrode array



Combinatorial inorganic coatings

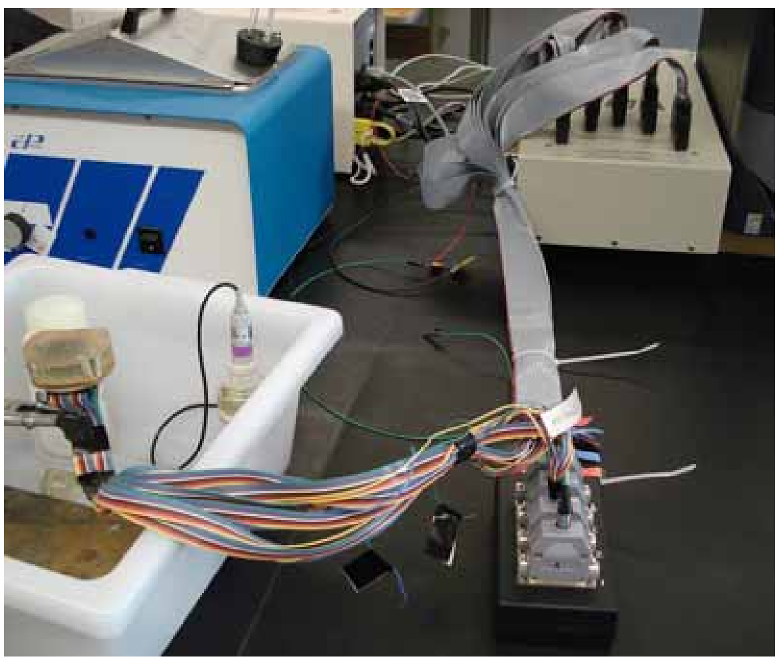
Micro-multielectrode analyser (MMA)

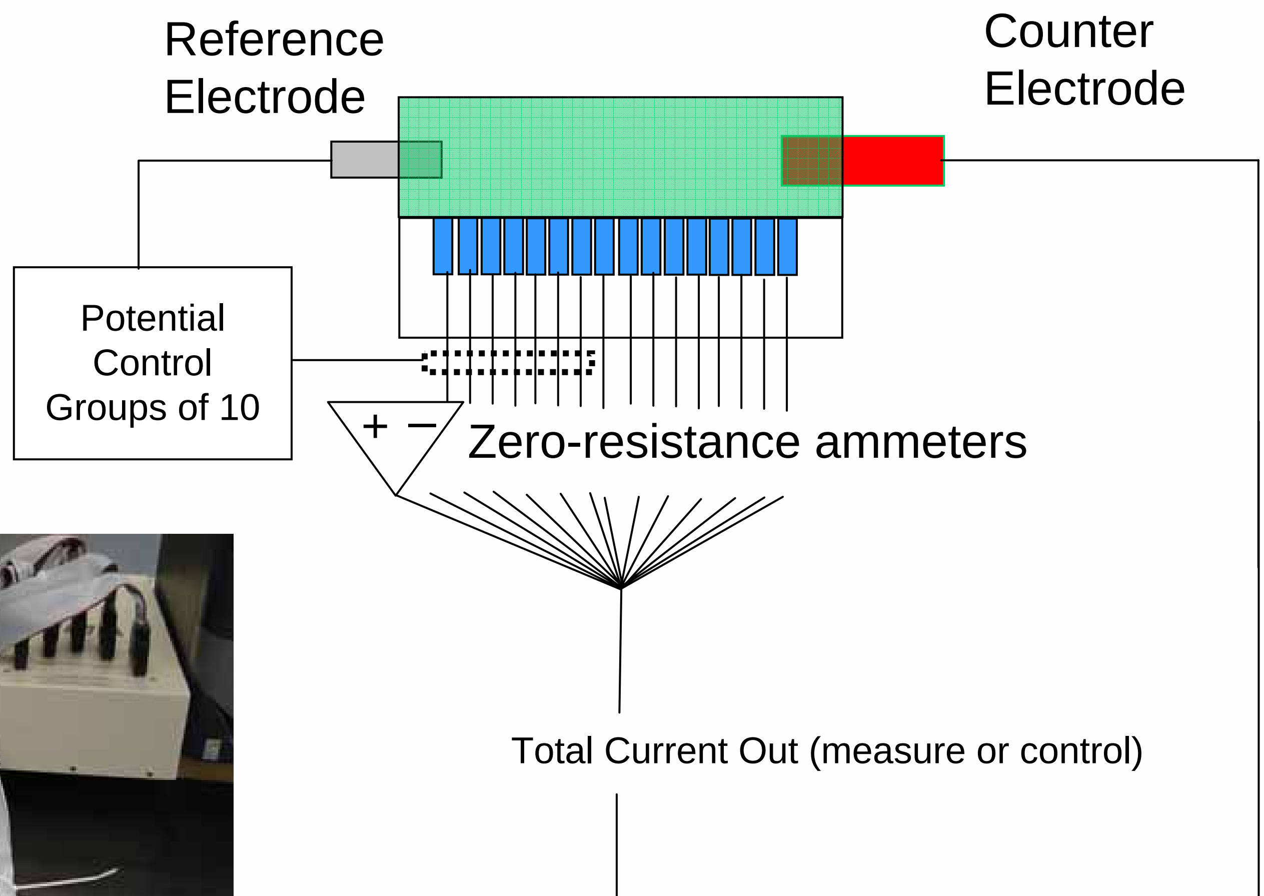
Current

Potential

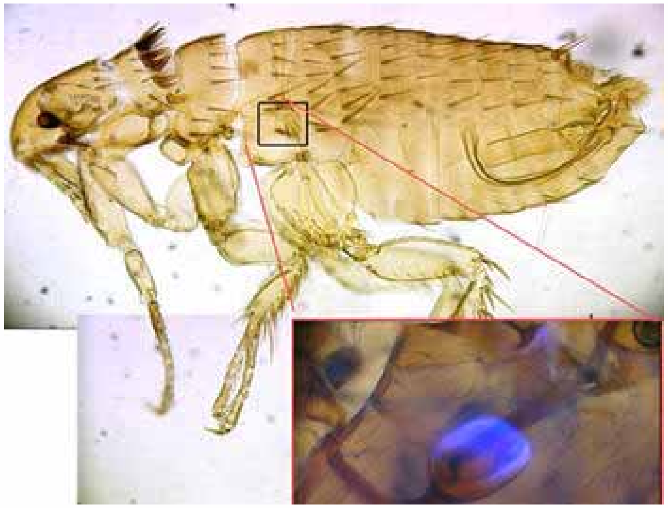
Impedance

100 Channels

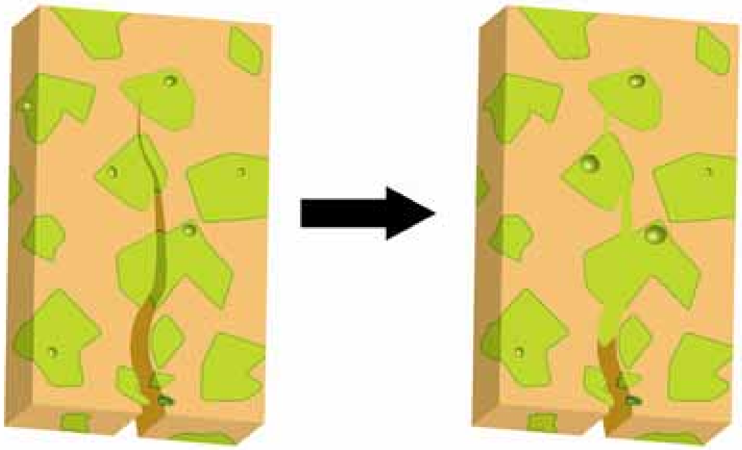




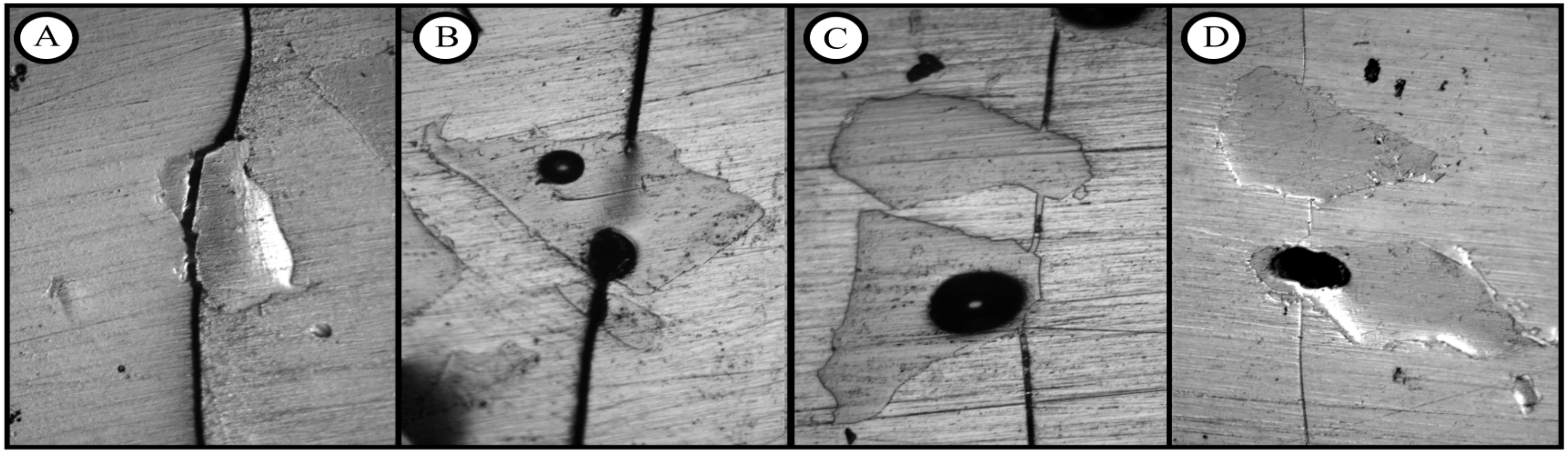
Bio-inspired materials and systems



Self Repair

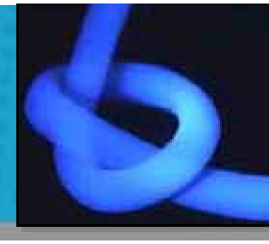


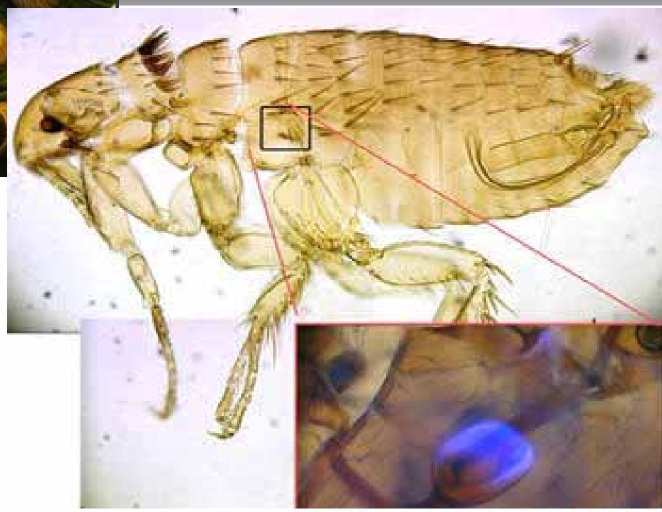
Polyethylene-co-methacrylic acid (EMAA) in Epoxy

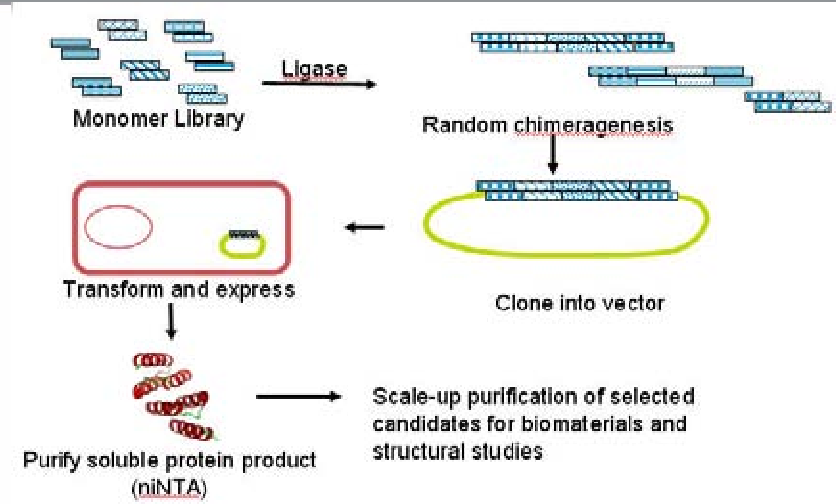


Adaptive and Responsive Materials

Resilin Bio-inspired







Results: **21 genetically distinct resilin modules generated**
Spider silk modules currently under development

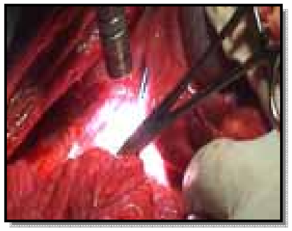
Protein-derived block copolymers (and hence unique biomaterials)

Generate information regarding the interplay between block copolymer sequence, length, and distribution on solubility, expression, protein structure and ultimately biomaterials properties to be used for future predictive modelling of new materials

Photopolymerised protein-based materials for biomedical applications

1. PhotoSeal

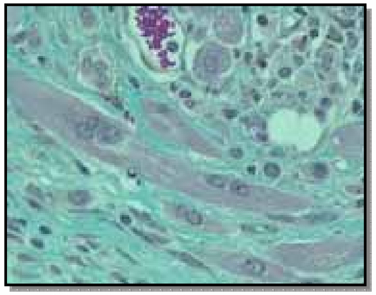
Surgical tissue sealant based on gelatin/fibrinogen



PhotoSeal applied as a "tissue glue"

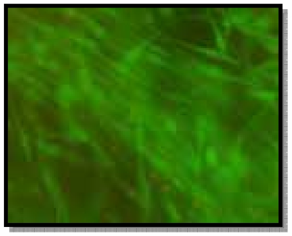
2. PhotoMatrix

Tissue engineering scaffolds based on extra-cellular matrix proteins



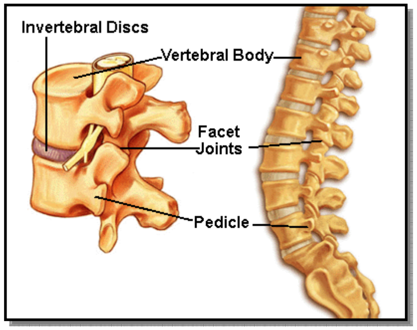
Muscle cells growing in PhotoMatrix foam scaffolds

In vivo



3. PhotoDisc

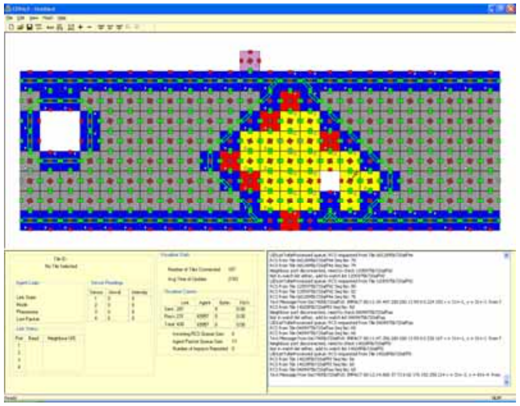
Unique bio-inspired elastomers for use in medicine (e.g. spinal disc) and industry (e.g. rubber)

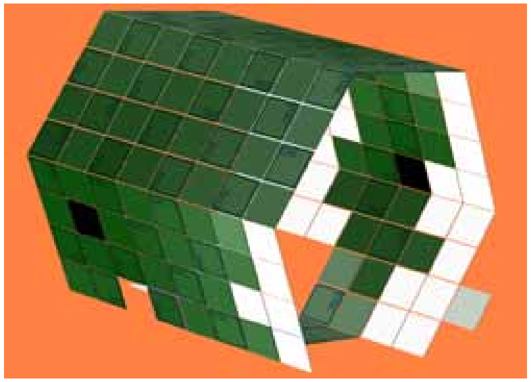


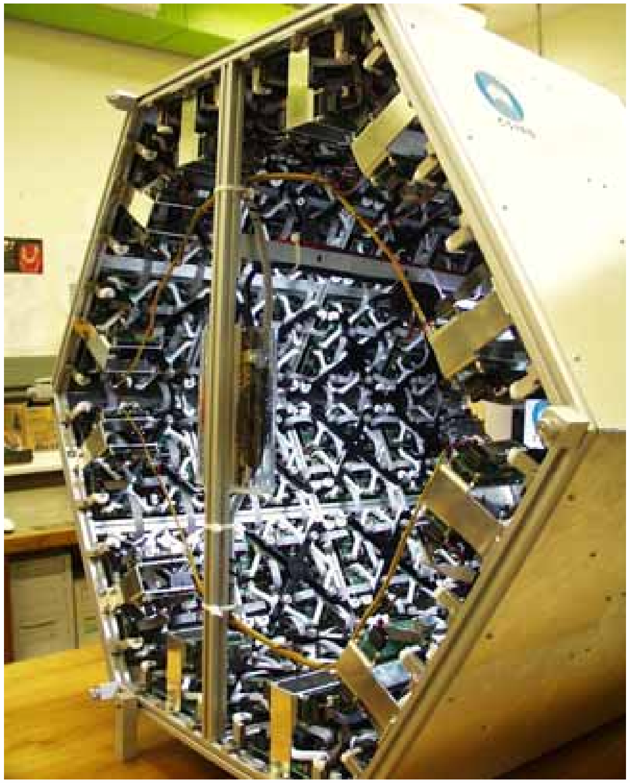
Recombinant resilin rubber

Distributed, intelligent systems

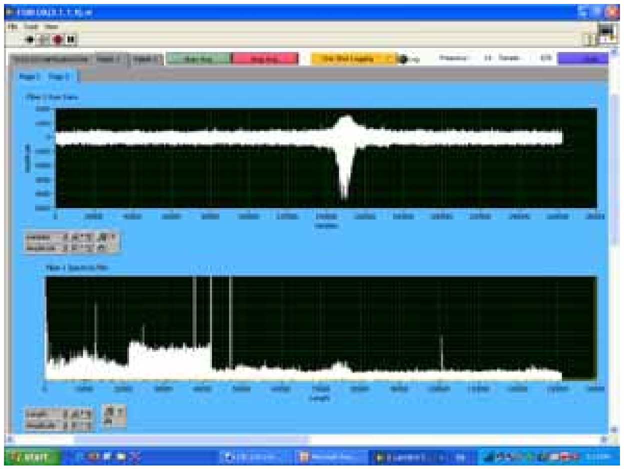
- **Structural health monitoring system**
  - The only SHM system in the world that employs a multi-agent self-organising architecture
  - Detects location and severity of impacts
  - Diagnosis, potential for prognosis
  - Secondary, mobile, autonomous agents

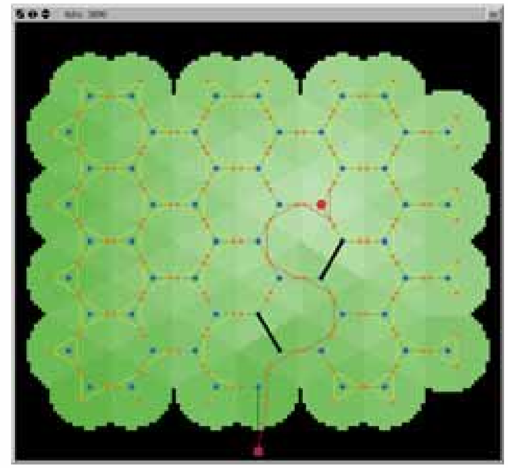


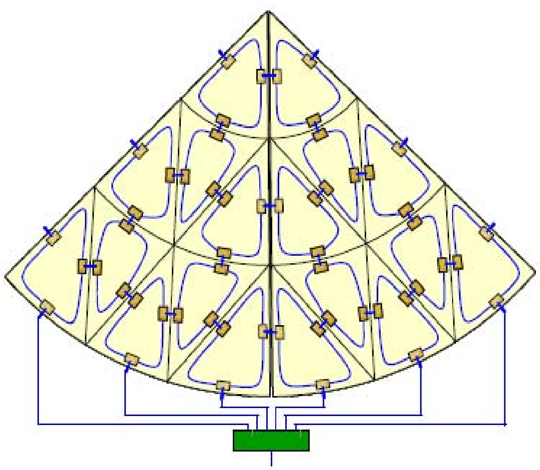


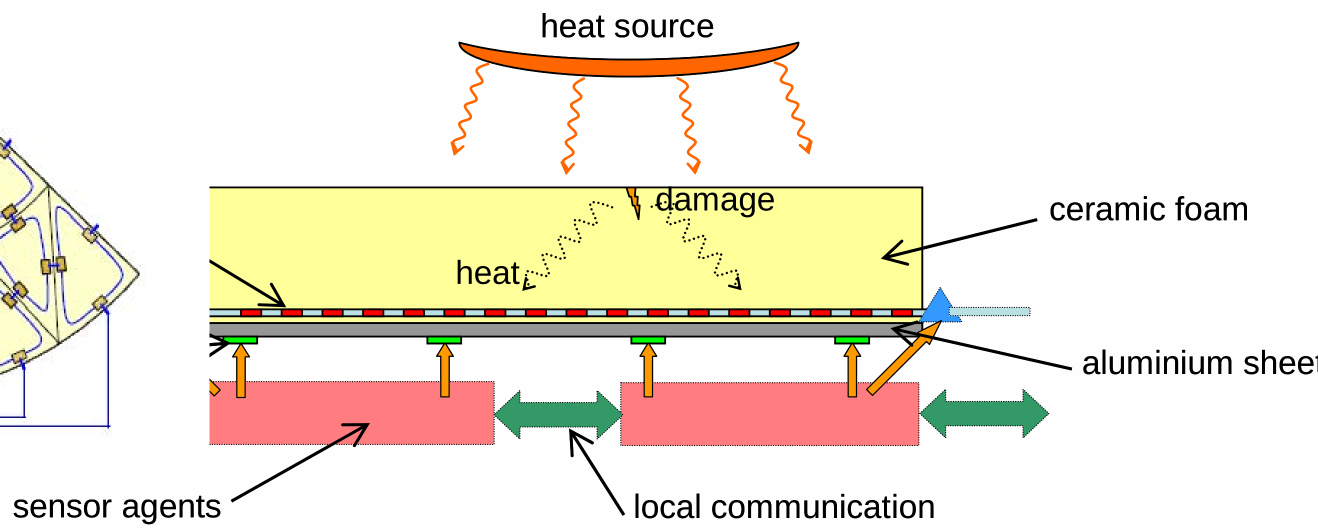


Optical fibre networking

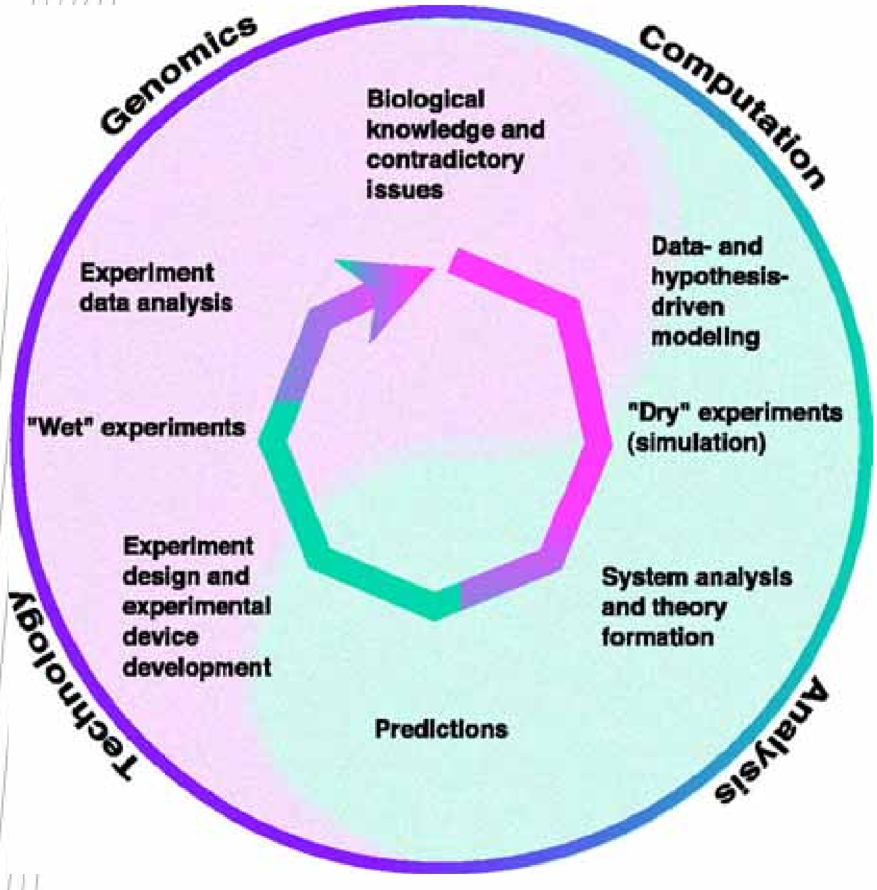


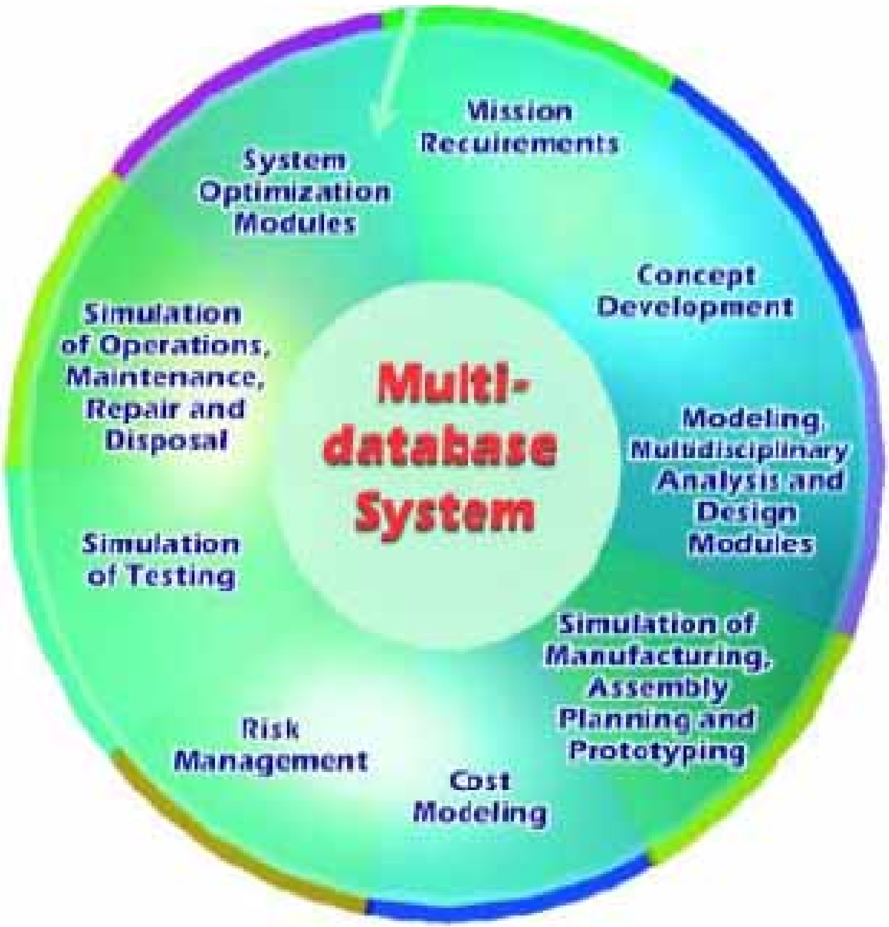






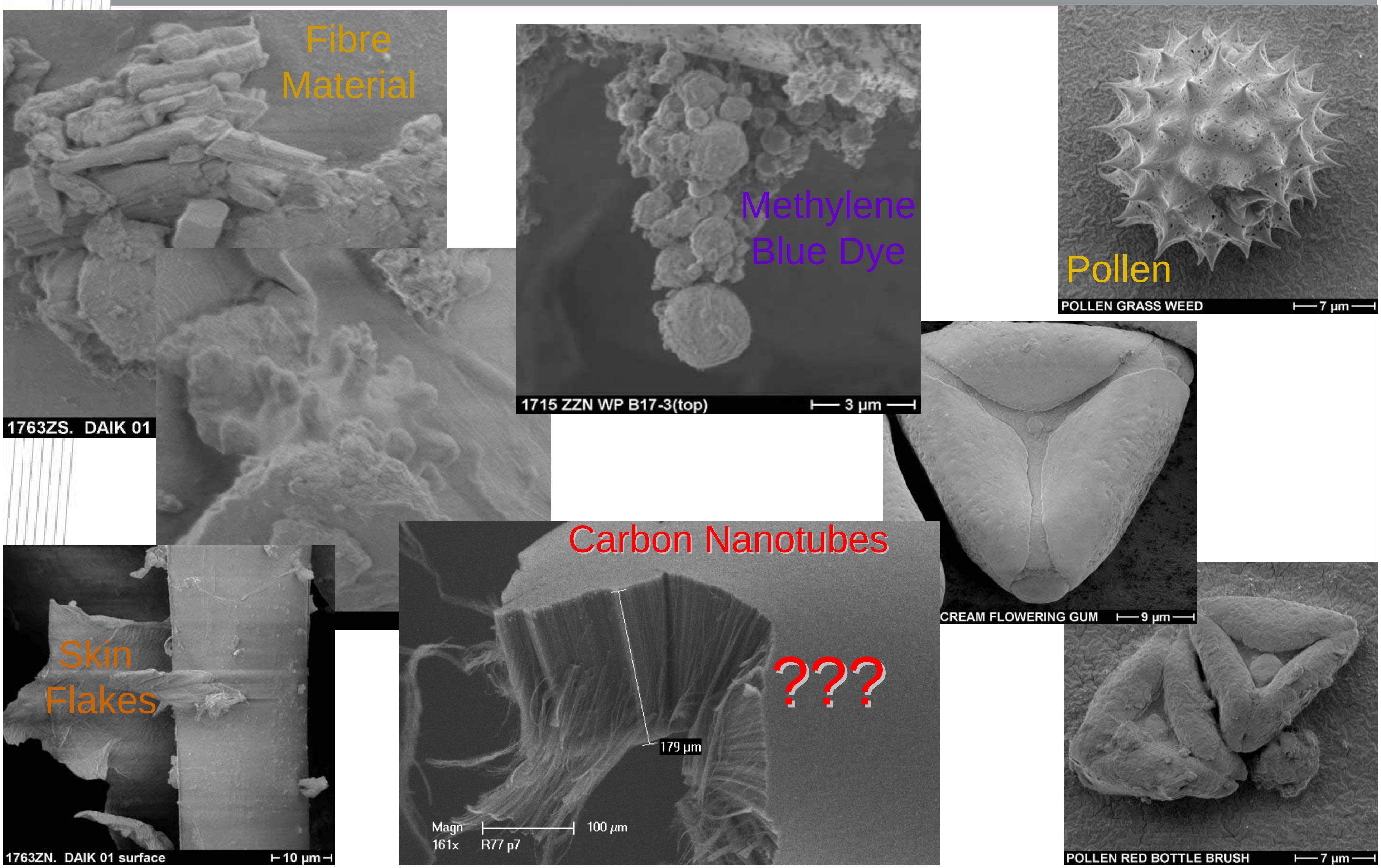
Materials Informatics





New and Nano Materials Safety

Workplace Monitoring for Carbon Nanotubes
Structure of Fine Particles



Workplace Detection and Measurement for CNT
Synthetic CNT Aerosol Test Duct

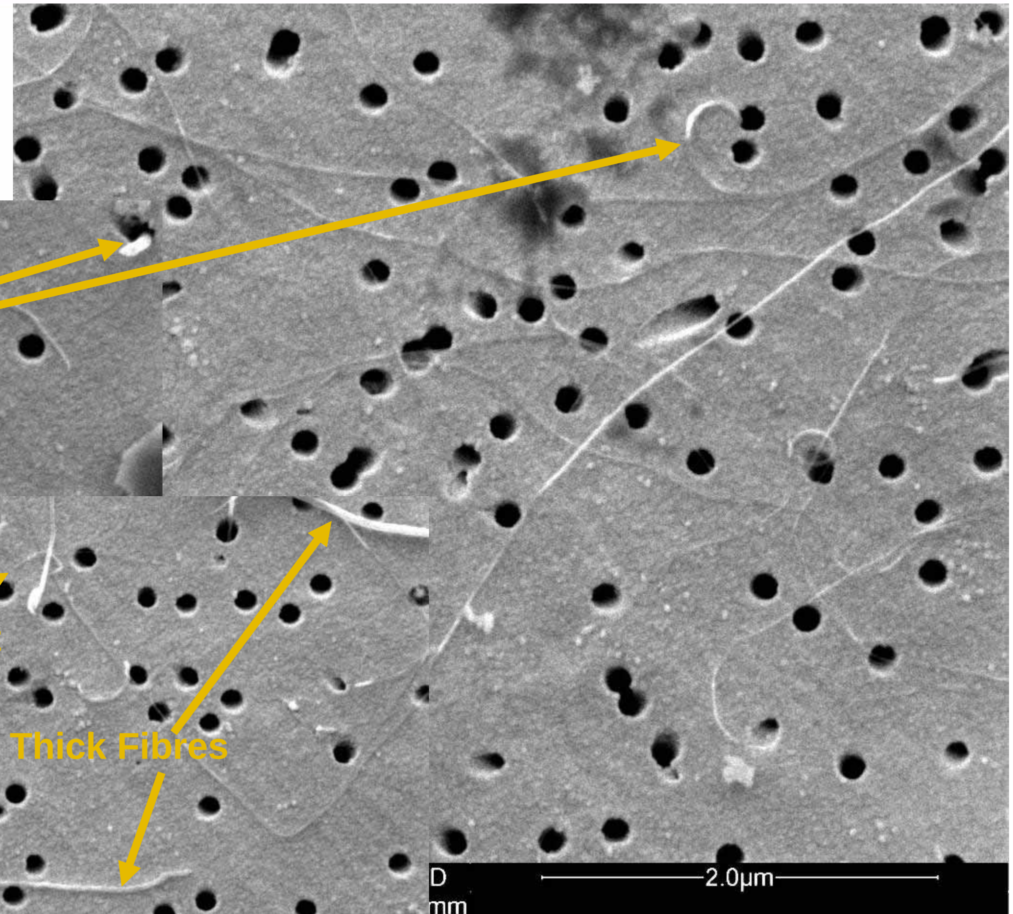


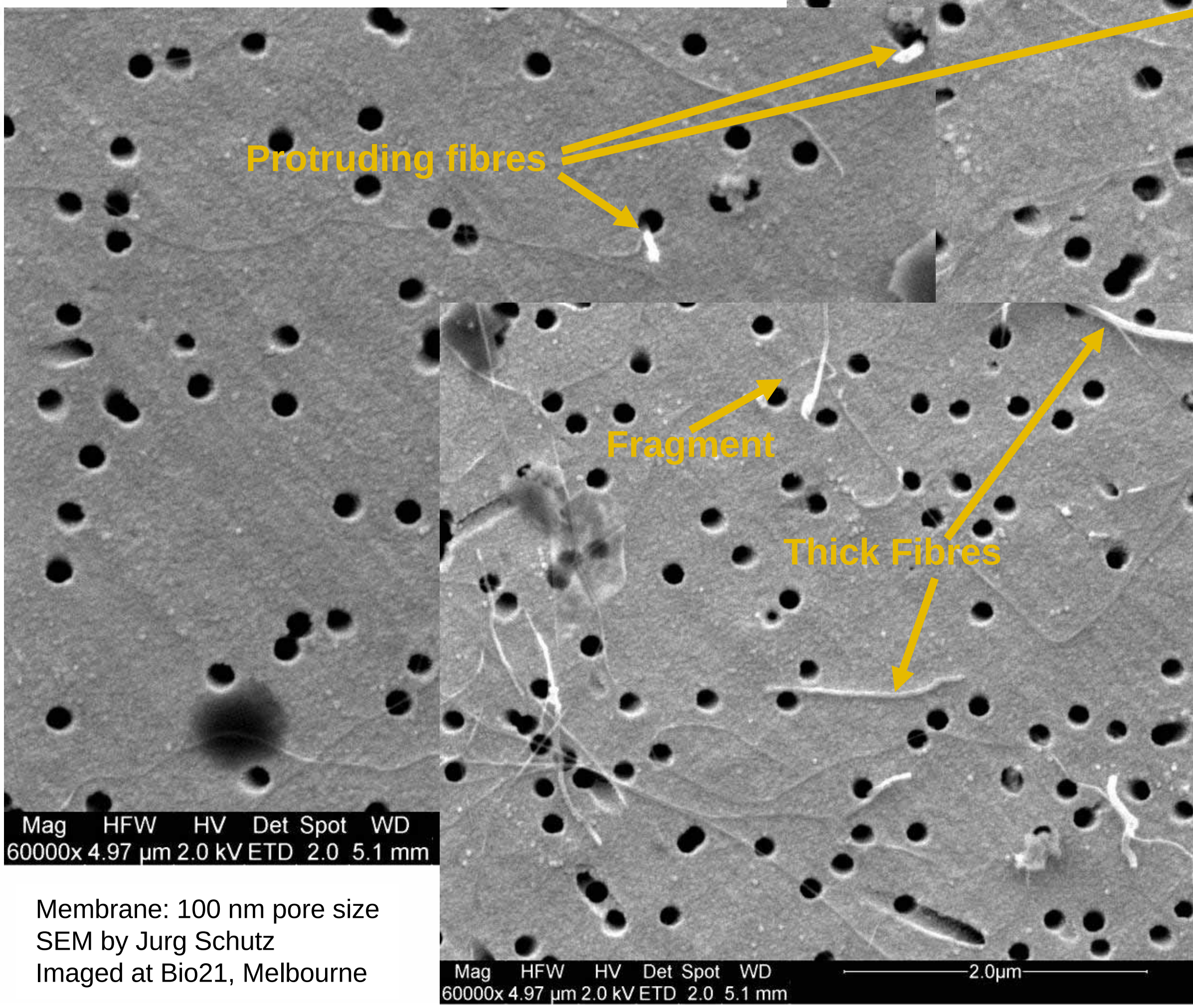
- **Provisions for Sampling**
  - Sampling Tubes
    - 2 Sets of 4 Tubes
  - Cowl Sampling
    - Exchangeable cowls
    - 25mm Membranes

- **Aerosol Generator**
  - Atomiser
    - KCl, NaCl in water; dryerite
    - CNT in Propan-2-ol; active coal
  - Options
    - Generator attached to base, which can be replaced by alternative generator system

Aerosol Sampling in CNT Laboratory
SEM Reference Samples (from CNT dispersion)

- **10nm Ø CNT from CPD, dispersed in Propan-2-ol, applied via fritted funnel**



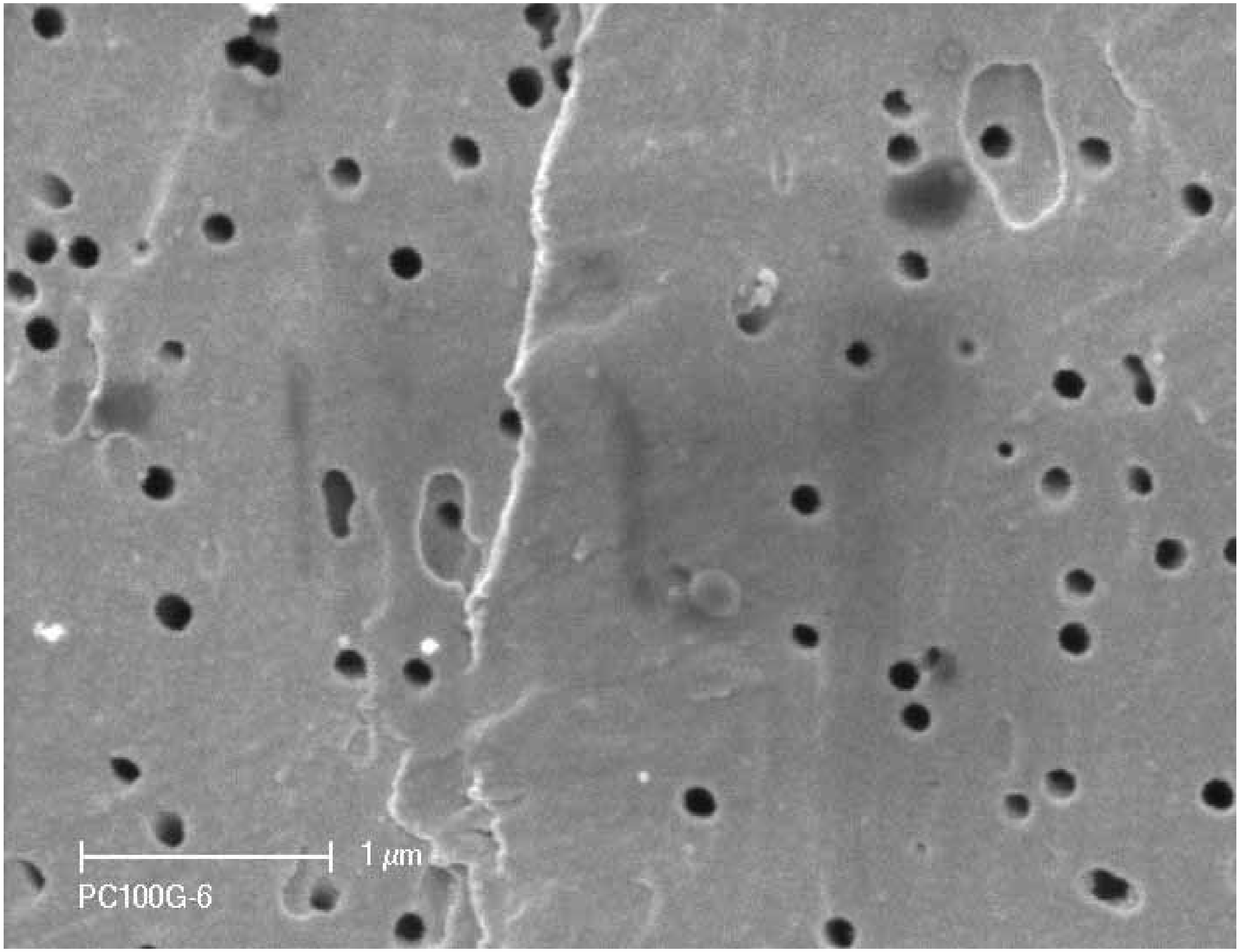


Membrane: 100 nm pore size
SEM by Jurg Schutz
Imaged at Bio21, Melbourne

- **Nominal: 7,000 Fibres / mm^2**
- **Counted: 333,000 Fibres / mm^2**

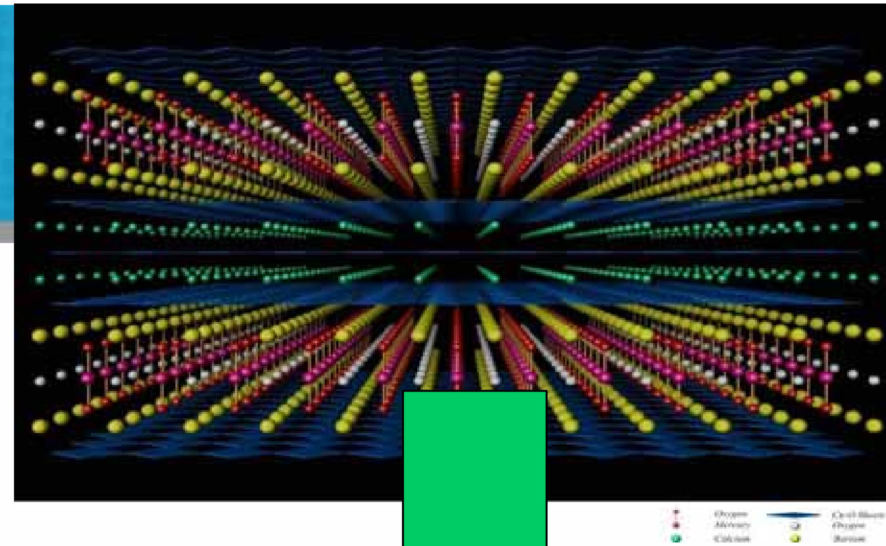
→ Fragmentation??

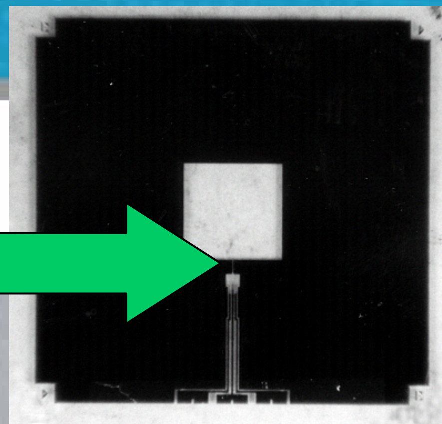
Aerosol Sampling in CNT Laboratory
Membrane From Sampling of 26 February 2009

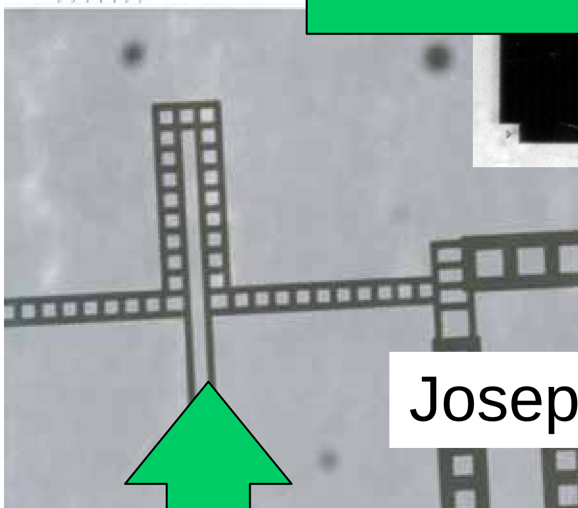


SEM image of membrane surface from sampling in CNT Laboratory at CSIRO on 26 February 2009

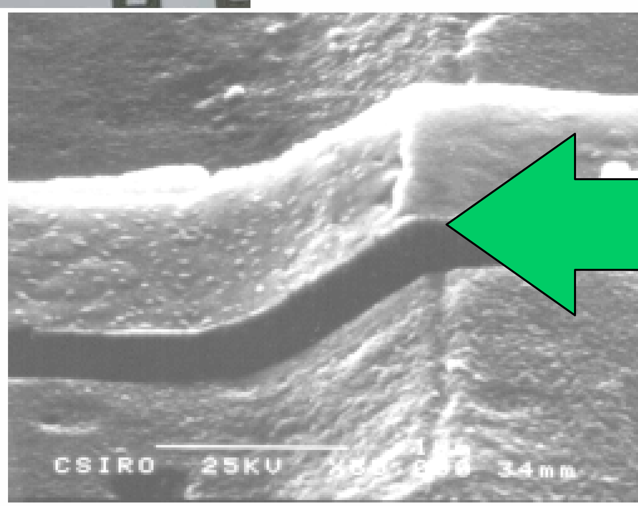
My own research area

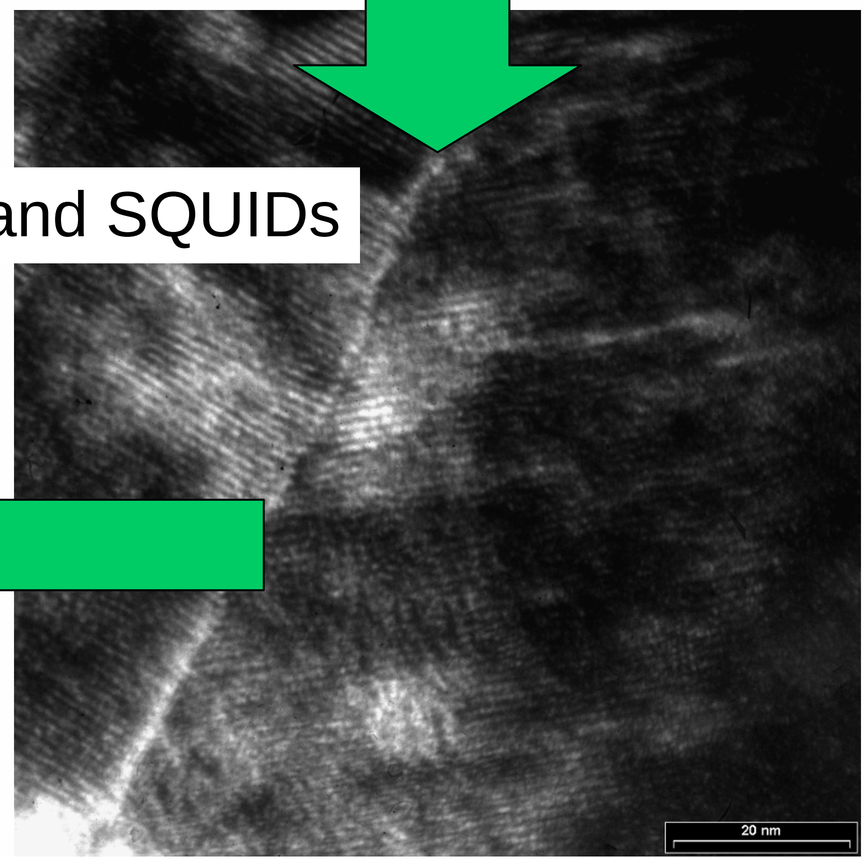






Josephson junctions and SQUIDs





Would like superconductivity to be bio-inspired……

ELSEVIER

Bioelectrochemistry and Bioenergetics 41 (1996) 27–30

Quantum mechanics: a breakthrough into biological system dynamics

M. Costato [a,c,*], M. Milani [b,c], L. Spinoglio [b]

[a] Dipartimento di Fisica, Università di Modena, Via Campi 213-a, I-41100 Modena, Italy
[b] Dipartimento di Fisica, Università di Milano, Via Celoria 16, I-20133 Milan, Italy
[c] Instituto Nazionale di Fisica della Materia (INFM), via dell'Acciaio 139, I-16153 Genoa, Italy

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Abstract

Superconductive and Josephson junction behaviour may be present in living cells. Positive experimental evidence is discussed. It is shown that the "Josephson junction paradigm" makes the connection possible between many different experimentally observed properties of living matter, allowing a further step towards a unitary framework for both physical and biological systems. Electromagnetic interaction plays a fundamental role. Superconductivity in biological systems can be demonstrated on theoretical grounds starting from a quantum microscopic approach to their dynamics.

Josephson-like behaviour can be expected (and is observed) in single cells at cytokinesis or for two nearby cells. Electromagnetic interaction between cells is a well-endowed candidate for driving intercellular communication and for organizing the transport of material through gap junctions established between adjacent cells.

Keywords: Cell interaction; Intercellular communication; Josephson junctions; Superconductivity

DNA proximity effect

Science 12 January 2001:
Vol. 291. no. 5502, pp. 280 - 282
DOI:
10.1126/science.291.5502.280

REPORTS

Proximity-Induced Superconductivity in DNA

A. Yu. Kasumov,[12*] M. Kociak,[1] S. Guéron,[1] B. Reulet,[1] V. T. Volkov,[2] D. V. Klinov,[3] H. Bouchiat[1]

Conductivity measurements on double-stranded DNA molecules deposited by a combing process across a submicron slit between rhenium/carbon metallic contacts reveal conduction to be ohmic between room temperature and 1 kelvin. The resistance per molecule is less than 100 kilohm and varies weakly with temperature. Below the superconducting transition temperature (1 kelvin) of the contacts, proximity-induced superconductivity is observed. These results imply that DNA molecules can be conducting down to millikelvin temperature and that phase coherence is maintained over several hundred nanometers.

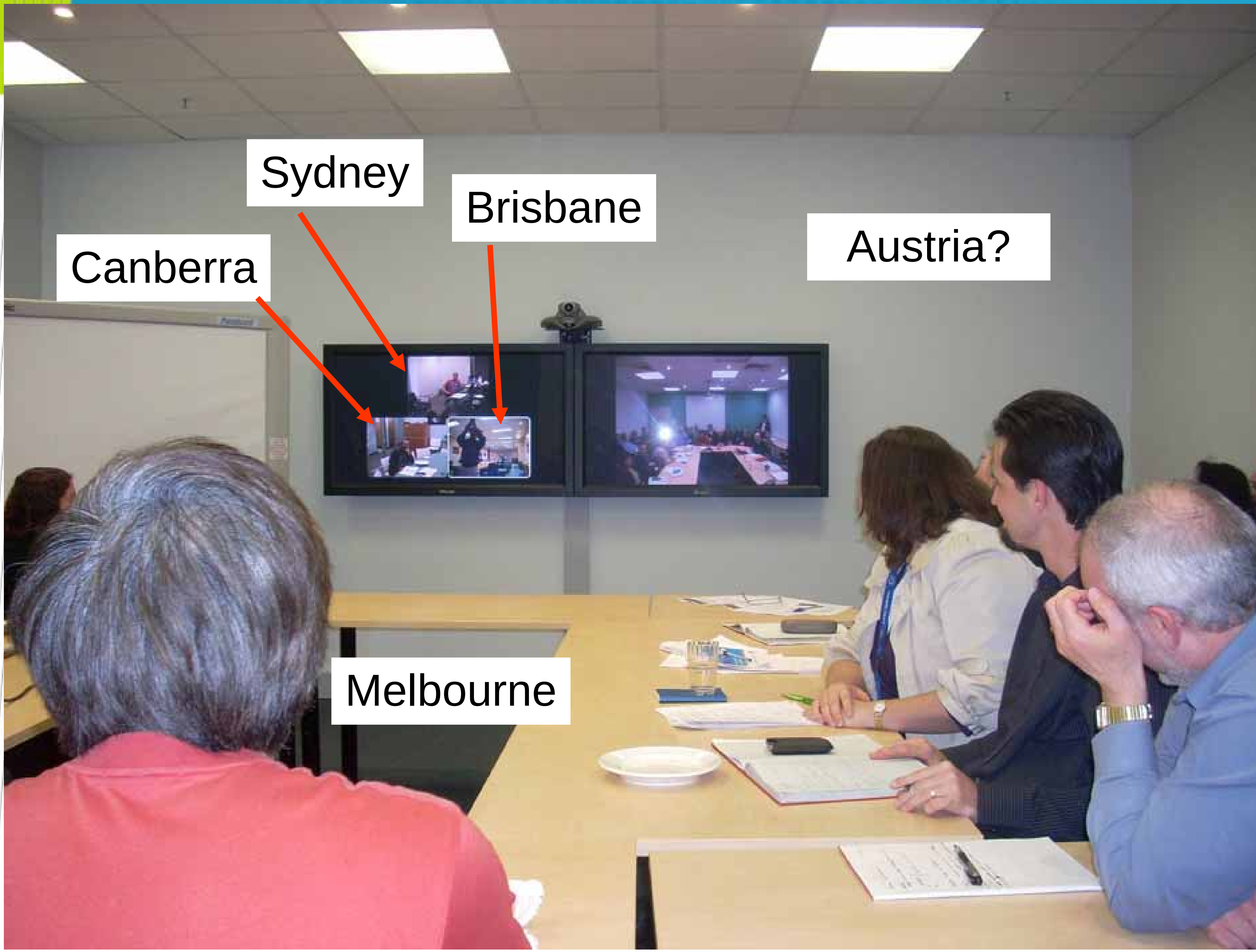
[1] Laboratoire de Physique des Solides, Associé au CNRS, Bât 510, Université Paris-Sud, 91405, Orsay, France.
[2] Institute of Microelectronics Technology and High Purity Materials, Russian Academy of Sciences, Chernogolovka 142432 Moscow Region, Russia.
[3] Shemyakin-Ovchinnikov Institute of Bioorganic Chemistry, Russian Academy of Sciences, Miklukho-Maklaya 16/10, Moscow 117871, Russia.
* Present address: Starlab, La tour de Freins, 555 rue Engeland 1180 Uclle, Brussels, Belgium.

Summary

- **CSIRO**
- **Wants to develop new materials**
  - Disparate properties
  - Increase rate of discovery
  - Reduce risks
    - Cost
    - Safety
  - Solve major problems

- **I hope to be bio-inspired for superconducting materials**

- **Good at collaborating across distances**


Sydney
Brisbane
Austria?
Canberra
Melbourne