Outputs of the EPSRC and BBSRC Chemical and Biochemical Solar Energy Conversion Workshop

Venue: Burleigh Court Loughborough University

Date held: 14th and 15th May 2007

Contents

Introduction

This report describes the outputs and recommendations of a workshop that was held in May 2007 at Burleigh Court, Loughborough University.

The initial idea for holding this workshop came from several horizon scanning activities. Firstly EPSRC was gauging areas of underpinning science that could be drawn into mainstream energy research. BBRSC had identified this area as one potentially yielding promising research. Finally the European Science Foundation (ESF), with input from leading UK researchers in this area, had published a report on this subject outlining the main technologies and the R&D issues associated with them. A meeting of EPSRC and BBSRC staff was held with Jim Barber (Imperial College) and Robin Perutz (York University) to discuss methods of stimulating research. A meeting was then held between EPSRC and BBSRC officers to find common ground. It was agreed that while much work was being done on photovoltaic research, the areas of overlap with the chemistry and biological science communities were not clear. It became clear that linkages between the various themes needed to be explored, new linkages made and existing linkages strengthened. It was decided to scope the area for possible cross-council activity. Therefore, a workshop was planned that brought together biologists, engineers, chemists, biochemists and materials scientists to identify the underpinning science that needs support in order to benefit energy research.

It was recognised that there are considerable portfolios of activity in this area already, notably two EPSRC SUPERGEN consortia; PV Materials for the 21st Century, and the Excitonic Solar Cells consortium; and the solar routes to hydrogen production project at Imperial College. These groups were invited to attend the workshop to ensure their input and to avoid potential omission or duplication in the outputs.

Prior to the workshop, BBSRC announced a call for expressions of interest in 'Capacity-Building Awards in Bioenergy Research'. This call was quite timely and the results of the call should be complementary to any activity that is supported as a result of this workshop.

The workshop began with three scene-setting presentations, the first from John Loughead of UKERC outlined the current energy debate. John detailed the state of UK and global power generation and noted that in order to meet future needs a range of power generation technologies will have to be harnessed. Of these, only solar has the potential to provide all of the energy required to plug the gap between the current power consumption of humankind (ca. 10 TW) and the power requirement projected for 2050 (ca. 20 TW).

The second presentation, by Robin Perutz of York University, summarised the role of solar energy and the technological challenges that solar energy faces. Robin outlined the principal technologies as photovoltaics, semiconductor-liquid junction cells, solar concentrators and photosynthesis. There are many technical challenges, but there are also other barriers to be overcome, such as basic communication between the different disciplines which often use very different terminology. We can envisage using solar power to generate electrical energy directly or to generate solar fuels. Photovoltaics are already in use for direct power generation, while semiconductor-liquid junction cells (Grätzel cells) are being manufactured on a small scale. Generation of solar fuels (H_2 +O_2 or CH_3OH +O_2) is exceptionally challenging because of the need for multi-electron redox processes. However, the example of photosynthesis demonstrates that it is feasible. Fuels such as hydrogen may be produced biologically (e.g. using hydrogenases) or as part of a tandem biological/artificial approach. Moreover, marked progress has been reported in bimimietic multielectron redox processes

Finally, Richard Cogdell introduced the ESF document and how it had evolved. An initial Department of Energy (DoE) workshop was held in the U.S. and produced a report available at http://www.sc.doe.gov/bes/reports/files/SEU_rpt.pdf. Following this a European workshop was held entitled "Harnessing Solar Energy for the Production of Clean Fuels" and produced a white paper: http://www.ssnmr.leidenuniv.nl/index.php.3?m=128.c=34. Following this, a second European meeting was held, also funded by the ESF, and as a result a Science Policy Briefing Paper was produced that is being discussed by the Council of the ESF. It is hoped that this paper will encourage both the ESF and the EU to initiate long-term research programs aimed at providing solar fuels.

The outputs of the ESF report "Harnessing Solar Energy for the Production of Clean Fuels" were used as the starting point for the discussions. A full copy of this report can be found at http://ewww.mpi-muelheim.mpg.de/bac/neuigkeiten/2006/10/31/cleansolarfuels.pdf . The fifteen themes outlined in this report were initially discussed by the delegates to determine whether they were an area of strength or weakness in the UK, and whether they were worth taking forward for more detailed discussion. From this initial assessment many of the themes were identified for development and were then grouped into broad, related themes. The areas that were identified were "Biological fuel production" "Electrochemical fuel production" and "First principles". Catalytic Processes and Materials were also identified as important themes but as they were cross-cutting and applied to all of the three identified areas it was agreed that they should be regarded as integral to all.

Themes:

Biological Fuel Production

Many research challenges were identified, mostly very tightly defined, for example;

- Enzyme properties
- Photosynthetic electron transfer
- Biological systems
- Collection and storage of H_2

However, some were broader in their technology requirements, including some interesting points relating to chemical engineering;

- Bio-refining and bio-processing
- Production of value-added biofuels and chemicals
- Conversion of biopolymers to biofuels

Additional areas included;

- Waste carbon usage
- Carbon delivery to bioreactors
- Photodamage resistance
- Environmental impact
- Land use.

The discussion highlighted short term and longer term challenges; in the shorter term the challenges are mostly the individual discipline areas whilst the longer term challenges involve the increasing collaboration between the disciplines while applying the fundamental sciences as they are better understood.

The economic and environmental aspects of biological fuel were also highlighted as an area where understanding needs to be improved. Some current conversion efficiencies are not competitive economically.

The issue of land use in the production of biofuels is an important consideration and is gaining attention. Biofuel crops are seen as displacing food crops, and use of food crops as fuel is leading to increased prices of staple foods. Algae are well noted as being able to grow in areas unsuitable for food production, thus the delegates noted that studies should be made on the potential for the use of marginal land and water, plus the use of waste water, in order to mitigate the impact on food production.

Delegates were not aware of any relevant environmental impact studies. Allied to this were public perception issues; will large scale use of biotechnology for fuel production, possibly involving genetic manipulation, be acceptable to the general public?

The overall costs are unknown not only the overall economics, where most of the studies are quite old, but also of the carbon balance. How carbon neutral are the various biofuels currently being produced?

Photoelectrochemical fuel production

There were many focused discipline base research issues;

- Better molecular oxidation catalysts
- Single and multiple electron photochemistry
- Computational modelling of mechanisms at the molecular level
- High temperature PV materials
- Hydrogen peroxide
- Chloride ion chemistry
- How to achieve O_2 evolution is still not clearly known
- Catalysis of electron transfer at a surface

There were also several cross-discipline issues;

- Studies of natural systems and the building of artificial analogues
- The need for nanostructuring to get transport carrier distances down to under 10nm
- In common with the biological theme there was a need for reactor engineering research
- Molecular assemblies that do more than one thing absorption/separation e-generation catalytic centre built in
- Stability issues
- Reduction of atmospheric CO_2 using this technology

Again the delegates highlighted the need for efficient systems, not just those that demonstrated proof of principle.

This theme identified a strong need for networking, bringing the various disciplines together to learn from each other, and to identify and roadmap a research strategy that can be followed by the whole community.

The discussion was wide ranging and covered many issues. The UK is seen to be doing internationally competitive research in this area, and there are many research challenges to address.

Some of the biggest challenges involve scale-up. Once a lab-based process is seen to work, low cost materials and substrates need to be developed, as well as membranes and other such product separation techniques.

The main element used as a photocatalyst is ruthenium, but this is a relatively scarce and expensive metal. Biomimetic systems would seek to use manganese as a substitute. Nature already uses Mn, which has multiple oxidation states, and much research needs to be done.

High temperature and high pressure photocatalyic reactors have specific challenges, they are not a very convenient method of water splitting. For real progress to be made in this area there needs to be a dialogue between chemists and reactor engineers.

The production of liquid fuels by this method is particularly applicable to transport. However, hydrogen purity is an issue for any fuel cell applications; separation and purification technologies need to be researched.

First principles

Again there were many discipline-based research challenges identified;

- Photon harvesting and charge separation
- Understanding the biological processes
- Surface science, e.g. catalysis, surface chemistry etc.
- Fundamentals to be worked out for biomimicry to produce robust molecules
- Molecular siting for the most efficient operation

Many of the problems will involve several disciplines such as research into self-assembled systems, biomimicry, self-repair mechanisms, liquid crystal chemistry, self-assembly of non-organic systems and self assembly of multiple functional materials.

There was again agreement that there is much expertise in the UK in this area, but there was much they could learn from related disciplines. They called for engagement with the photovoltaic community to discuss methodologies etc, and to bring related communities into the field. The discussion highlighted that there is now lots of new molecular information that is moving this area forward. Biomimicry for self-assembly was advocated as a particular challenge, as current experimental methods use very crude self-assembly whereas biology produces some very complex structures. The challenge is to identify the individual challenges that can be tackled either separately or in conjunction.

This theme highlighted strongly the need for networking to bring the various disciplines together; summer schools were suggested as a means of getting researchers, especially project students, together and to expose them to the broader challenges of this research field.

Conclusions and Recommendations.

The main messages of the delegates were:

- The basic science of solar energy conversion is one **the** grand challenges facing energy research
- Solar energy has the potential to provide distributed power and fuel on a terawatt scale (worldwide) if the scientific challenges can be overcome
- The area as a whole requires a co-ordinated and sustained research effort
- The UK is well placed to address these challenges having much world renowned expertise in most of the areas discussed
- It was recognised that there is a real need for cross-council action in this area
- The workshop itself is the first stage of this process

- The outputs from the workshop will form the basis for future activity
- Given the necessary organisation and support, the UK has the capability to become a leader in this area and has the potential to strongly benefit the UK economy
- Researchers in Chemistry, Physics, Biology and Engineering are working in this area already and need support to work together

The delegates recommended the following:

The creation of a network to bring researchers from across the disciplines and representatives from industry together regularly to discuss the issues and to form new links, should be the first priority. The delegates identified the BBSRC bioenergy call as an immediate opportunity to make some aspects of this happen.

A road-mapping exercise should be undertaken to define the landscape in which researchers will be working. Similar roadmaps exist in other disciplines (e.g. the Hydrogen economy roadmap published by the DoE) and procedures for doing this are well understood. This roadmap will identify the deliverable milestones that would be the backbone of any long term research activity.

Capacity issues were raised as a point of concern: currently, there are few people working in the field considering its great potential. Capacity should be addressed as part of any activity proposed and should be integral to both the proposed network and research programme. The UK expertise in this area would benefit from the opportunity to learn from related disciplines and there should be engagement across the photovoltaic, photochemical and photobiological communities to discuss methodologies etc, There should also be opportunities to bring researchers working in related communities into the field, such as those working in metal oxides or in molecular self-assembly.

Since such projects are needed in the long term, the creation of a network group or sub-group of young researchers undertaking activities that encourage schoolchildren to study the disciplines associated with this area should be encouraged.

A targeted activity that addresses the above points should be initiated. Any such activity should be constructed carefully to complement existing activities, have clearly defined objectives and milestones (identified from the road-mapping exercise), and should seek to bring the communities working in this area together to encourage cross-disciplinary research. Research support should be targeted at a wider community than at present.

The delegates also wanted to see specific energy fellowships being awarded.

Research Councils' Observations:

The workshop was well attended with good representation from four academic disciplines. Discussion was well informed and encouraged the sharing of ideas and knowledge between the disciplines. It appears that solar energy research would benefit from an activity that would provide an umbrella for the various disciplines and the research that they currently undertake, and provide a mechanism for cross-discipline learning and generation of new research ideas.

Any network, or other large scale co-ordinated activity, organised in solar energy should also be inclusive of existing effort and seek to strengthen the ties between research groups. It should go further than this and actively seek to make contact with researchers who work in related disciplines and bring them into the field.

There are clearly defined research challenges identified from this workshop, and there are many possible activities that could be undertaken. Given the constraints on funding, duplication of research effort must be avoided. As existing consortia are already attacking many of the research challenges, any new activity **must** complement and build upon the work that is already being supported. Additionally linkages must be made between any new activities, and with interested research groups that work in related disciplines that may be new to the area. By its very nature any new activity should be an inclusive activity that brings together biologists, chemists, physicists and engineers working together in an integrated and flexible way, and boundary issues between the research council remits must be avoided.

Annex

Transcripts of the workshop flip charts and Proformas

BIOLOGICAL PROCESSES

10. Theme: (Anaerobic) H_2 Production

UK Capability	Research Challenges	Involvement needed	Timescale
Anaerobic H_2 production - very little Jim Barber et al (Chlarydoronos Rhodobacter)	Optimisation and reactor design Optimisation of H_2 production efficiency Gen mod of organisms	Academic Engineers and Industrial input	Relatively short - 5 years?
Overseas capability UK links Not much! EU consortium Work going on - not anaerobic (part of BP initiative → Berkeley, US/DOE)	Molecular basis of hydrogenase activity Containment Scaling-up Capacity-building in UK - RAID profile Integration with other technologies (hybrid schemes) (what to do on a gloomy day!)	Combine with 9 - Lauri Peter Networking - who is doing this????	

BALLOT BOX	3 dots

11. Theme: Design of Photosynthetic Cell Factors

UK Capability	Research Challenges	Involvement needed	Timescale
UK has strong/good: - higher plants - microbiology Bioprocess intensification and cell manipulation **Overseas capability UK links** Manipulation of tropical plants (not a big problem)	Designing 'minimal cell' - may be unnecessary and may not work Manipulation of cells - more feasible Higher plants - growth on marginal land (to avoid use of arable land) Bioreactor development - physiological stress control at micro-scale High throughput screening (plants and microbes)	Industry not likely to fund this - needs Research Council funds University spin-outs	Within 5 years (research) 5+ years development and implementation

BALLOT BOX	6 dots

1. Theme: Biological Blueprints for Solar Hydrogen Production from Water

UK Capability	Research Challenges	Involvement needed	Timescale
Good at present, but needs significant investment now (water splitting). Recruitment of senior personnel	Details of water splitting still unclear	Basic research needed on water splitting	5-10 years
Leading UK groups working on H_2 production (hydrodgenase)	May not need to understand full mechanism to exploit water splitting reaction	Utilise photo-synthetic organisms which already do this for eg H_2 production	5-10 years
Overseas capability UK links	Lots of useful information to be gained from looking at hydrodgenase - basic research on properties and engineering	Basic research on H_2 production	5-10 years
Arizona - water splitting Colorado - H_2 production Mülheim - water splitting Berlin	Mimicking water splitting reaction very difficult (biomimick)	Basic research needed first	Unclear basic research needed first *Catalytic reaction on surface area still unclear. That diverts the focus a bit*

BALLOT BOX	12 dots

9. **Theme: Solar H_2 and CO_2 Biofuels Green Algae**

UK Capability	Research Challenges	Involvement needed	Timescale
Good skill base	Re-engineering organisms (GM-issues) ecological issue	Engineers and Biologists talking	Lab scale 5 years to ∞
Strong basic science Lots of interest in applied research in this area. Not much research at the moment	Controlling environment, and stresses - scale effects (micro-scale) Oxygen tolerant hydrogenases Organism stability		Long term
Overseas capability UK links Large amount of US work in this area. Everyone except UK!	Selecting for algae with high HC content and growth	Basic research metabolism	5-10 years
	GM organisms	Engineers and biologists and industry	NOW
If Britain//Europe are serious about solar fuel research, all aspects/technologies will have to be explored. What appears to be missing from this meeting is higher plant biofuel production. The major issue here is where will these higher plant biofuels be grown? With increasing pressure on arable land for food production, marginal lands will have to be used. So an additional question is "what limits plant production in marginal lands"?	Use of FEW gases (capturing CO_2) Cost effective processing/reactors Distributed reactors Scale up of Bioreactors Exploiting marine environment/salt water What about higher plants carbon biofuels?		5-10 years *Should be amalgamated with biological blueprints for solar hydrogen*

BBSRC funds research in crop science, all aspects of plant biology and interdisciplinary science should be opportunities….

BALLOT BOX	24 dots

BIOLOGICAL PROCESSES

Solution	Barrier to Progress
Bacteria	Conversion rate CO_2
CO_2 - microbial/algal - focus on macro - micro delivery - plants - stress/slomata	Technology available but requires adaptation
Light-efficient usage and screen biological systems	Assessment of materials development of new technology R&D
Land - assess open/closed bioreaction (algae) Performance on marginal land (plants)	Assessment of performance (not known) Understanding of basic principles
Biological systems - assess materials	Screening of biological resource for specific 'habitat' Public perception….
Water and nutrients - assess systems and impact of nutrients	Lack of understanding funding
Carbon polymers → biofuels Bioprocessing Bioengineering	No efficient system for C → biofuel production other than fermentation

Prioritised Research Challenges **Theme: Biological Processes**		
Challenge	Required Activity	Who?
1. Co_2 delivery Macro - source, conc, delv to 'reactors' Micro - delivery to 'biocell'	Engineering focus with input from biologist Materials science	Biologists with engineers RC-funded Industry involved at early stage
2. Light - efficient usage, photodamage	Engineering 'bioreactors' and materials, input from biologists	Engineers with biologists
3. Land where? Algae - closed bioreactor - open bioreactors Plant - Marginal law	Assess performance in environment - engineers and biologists	Engineers and biologists
4. Biological systems algae and plants	Screen material bioengineering Pollutant tolerance (waste input) Fundamental biological research 'Ecology' with open systems	Biologists
Bottleneck long-term 5. Water and nutrie Algae and plant: understanding	Assess impact of nutrient supplementation on yield Saline/fresh/waste Manipulated osmosis Insitu fertilisation	Biologists

Biology is probably more important than engineering

Targeted funding for biology, chemistry and engineering

Not just algae/plants also bacteria/biological (cell) components)

Microbial ecology of algae systems w/involvement of biologists and engineers very needed

BIOLOGICAL HYDROGEN PRODUCTION

Prioritised Research Challenges **Theme: Biological Processes**		
Challenge	Required Activity	Who?
Enzyme properties Hydrogenose, nitrogenose etc	Crystalography Spectroscopy (GPR…) Theory	Co-ordinated teams of chemists/biochemists/spectroscopists (UK expertise currently fragmented)
Redirecting photosynthetic electron transfer	Molecular biology Physiology Spectroscopy Systems biology	Skills HGRC in the UK funding, direction and co-ordination required….
Semi-synthetic systems - microbial fuel cells	Electrochemistry and biology	Focussed effort
Collection and storage of H_2 from bioreactors	Engineering and biology	
Waste carbon sources for anaerobic H_2 producers	Collaboration between academics and industry	
Microbial ecology consortia etc		

Also important for algae/bacterial

Raw material source is limited

H_2 storage is a real and important barrier

H_2 has to be used in-situ for it to be viable

Prioritised Research Challenges **Theme: Biological Processes**		
Challenge	Required Activity	Who?
Bioprocessing/ Biorefining	Bioengineering Chemical engineers Process engineers	RC-funded Possibly industry
'Value-added' biofuels/biochemicals (pharmaceuticals, fine chemicals, polymer precursors)	Biological research/engineering Cost analysis	Biologists RC-funded Industry
CO_2 sequestration - within remit?	?	
Carbon polymers to biofuels	Intensive Research on biocatalysis Chemical catalysis	Chemists Biologists Chemical Engineers

MATERIALS

6. Theme: Smart Materials/Responsive Materials (How to copy nature and control self-assembly)

In self assembly: controlled **UK Capability**	**Research Challenges**	**Involvement needed**	**Timescale**
Synthetic chem strong → but not focused towards self assembly	Supramolecular chemistry still works on a much smaller scale tens of molecules - not at stage of building large ordered structures	Very hard to get funded when working at biology/physics/chemistry interfaces	? Now ↓
Good nanotechnology	→ Scale up to get order transferred from picoscale → macroscale	Old boundaries no longer relevant Fund more blue sky cross disciplinary research	Long term funding!
SOMS and surface science centres	Need the spectroscopies to probe things occurring on different length scales and at surfaces	In-depth workshops on special areas → and funding to allow networks that result to do the research	
Overseas capability UK links Netherlands strong Strasbourg	Need <u>control</u>		
The whole "Nano" community falls under this topic and is under-represented here!	There is a <u>sub-theme</u>		

BALLOT BOX	7 dots

Theme 7: Energy Storing PV Devices

UK Capability	**Research Challenges**	**Involvement needed**	**Timescale**
Regenysis system (what happened to it?) Latent know-how eg electronics industry	Need a wider range storage options - relatively Why membranes? Combine RZR plastic solar cell with plastic batteries - but….. focus on higher efficient cells first Limitations on redox systems that fit a) energy levels; b) environment Materials challenge	Rethink this topic	ASAP This should be combined with photoelectrochemical fuel generation - very similar
Overseas capability UK links ?			

BALLOT BOX	3 dots

5. Theme 5: Materials for High Efficiency Low Cost PV

UK Capability	Research Challenges	Involvement needed	Timescale
Industry - yes, varies, excellent potential (eg strong support for recent Carbon Trust event) Academic - excellent (PV) (internationally - leading aspects) (internationally - comparative in others)	Improve links with biomimetic/self-organisation community Develop links outward from PV to battery and/or fuel cell technologies → focus and leadership may be provided from this existing area to bring in chemists, biochemists etc (NB See output from UKERC PV Roadmapping Exercise 2006)		
Overseas capability UK links EU programmes (very strong links)			

Combine Themes 5, 6, 7

This topic should be <u>excluded</u>. Overlap in PV Supergen and materials for energy too strong

Not for those of us not included!! - Agree!!

Strong overlap with existing Supergen consortia

This is an area that requires the priority

What would be the outcome of this survey?

BALLOT BOX	9 dots

14. Theme: 14 Characterisation of Integrated Functional Architectures of Cat Devices Using Novel Technologies

UK Capability	**Research Challenges**	**Involvement needed**	**Timescale**
Many techniques well represented but not addressing key solar challenge. Need commitment to problem not just central facilities **Overseas capability UK links** Outstanding capability of techniques similar but much more focused on solar problems Combine Themes 14, 15 A sub-sub theme! Absorb into main theme(s)	Theoretical techniques eg excited states. Theory to inform expt Investigate nanoscale materials under operating conditions at high spatial resolution Membrane proteins - isolation, expression, crystallisation Development of Lane methods Addressing issues and photodamage and studying with minimum damage	Collaborative project with techniques people as well as systems people Large scale long term	Long term - flexibility Needs to be deducted to problem not a general service for all science

BALLOT BOX	9 dots

PHOTOELECTROCHEMICAL FUEL PRODUCTION

Prioritised Research Challenges

Theme: Biological Processes

Challenge	Required Activity	Who?
New materials: - photostable materials - catalysts - hetrostructures/ nanomorphology/ nanoenvironment - ???? gap engineering	Co-ordination Networking (PEC - net UK) - define the problem - identify the stakeholders - set-up <u>inclusive</u> framework - establish critical mass	 Academic and industrial stakeholders
Recombination - excitonic Complex reactions	Industrial involvement International contacts - workshops (ev/day) - obtain funding for WS	 SCOPING WORKSHOP
Product separation Alternative products CH_2, H_2O_2 Coupling molecular light absorbers (that drive H_2O oxidation reaction) with charge transport MOs	Sufficient funding Publicity Stimulate collaboration at the chemistry/working interface	→ EPSRC/BBSRC

8. **Theme: Photoelectrochemical Fuel Production**

UK Capability	**Research Challenges**	**Involvement needed**	**Timescale**
Academic: Good potential but not focused on issue Industry: Small SME base - but strong internationally Strong in fuel cells	Efficient, stable catalyst for multi electron transfer for H_2O oxidation Integration with light absorbing/PV component Materials discovery for inorganic photoelectrodes (nanostructuring) Identification of optimum systems approach (input from PV, fuel cell …. Communities) Fundamental directional studies CO_2 reduction	Bring in metal organic/inorganic catalyst community and biomimetic research Synthesis and computational Electrochemical engineering	As in ESF document The main message of the workshop I think is that there needs to be a dedicated programme which addresses the three main themes recommended by the ESF - see page 3 I think funding under this should go to collaborations which integrate the components of a whole system. This would provide best value for money No use made of back casting - deciding what your end goal is, then tracking backwards to establish the critical and alternative paths. This then integrates all necessary work into a whole effort in an efficient way Important to prove materials science input combining photo and electric fields together with the catalyst. This is best done in structured microreactors
Overseas capability UK links Overseas strong in Japan, NL, Australia, Switz, US Links low inhibited by lack of UK focus and funding			

BALLOT BOX	24 dots

PEC - PROCESSES

- Exciton generation
- Charge separation
- Charge transport
- Redox reaction

PROBLEMS

- Recombination/competing back/side - reactions
- Photo-stability of materials
- Change accumulation
- Nano-morphology and evironment
- New materials, catalysts

FIRST PRINCIPLES

Prioritised Research Challenges

Theme: Photons → Charge Separation → Catalysis Biomemetic Approach

Challenge	Required Activity	Who?
1. Integrate oxidising (hole) and reducing (electron) parts into a stable molecular device for catalytic reaction 2. Self-assembly as a means of improving org or polymer vs biomemetic PVs based on principles of self-organisation and assembly 3. Get right people working together o keeping them at it in the long term 5 years renewable for a further 5	Consortium - multiple skills eg biochem, surface sci, photophysics, chem. Synthesis, theory, high level, spectroscopy Pre-consortium - for networking building Identifying the right people with top rate skills who are passionate about the problem and will work effectively together Spanning the disciplines Discipline hopping Summer School Fast track start up grants to facilitate network Accept risk - internet reviewers This would be a cross-Council (EPSRC/BBSRC) activity + STFC Mechanisms for co-ordination and triaging project along the way	All present interested Flavell (metal oxide surface science) Raval (self-assembly at surfaces) McGrady (electronic structure) Xiao Guo (biointerface phenomena) Herz (org semicon and ultrafast spc) Robertson (electro active molecules) Weinstein (molecular charge separation transient spec) Cogdell (beautiful bio structures photobiol) Tucker (superamol synthesis) Beddard (ultrafast spec energy and electron transfer) Durrant (photochemistry and devices) Perutz (photochemistry synth of change - separated) Harry Anderson (Oxford Synth) Neil Hunter (Sheffield, ind. bio.) Chris Hunter (Sheffield, synth)

2. Theme: Photosynthetic Antennae

UK Capability	Research Challenges	Involvement needed	Timescale
Strong- biochem, structure, function - Nanotechnology - Supramolecular synthetic chemistry Organic semiconductors - spin-outs and industrial Mainly academic Femtosecond and fast kinetics - small UK community **Overseas capability UK links** US - femtosecond and laser expertise and equipment	Get required communities - chemists - biochemists - etc Learning how to produce ordered arrays of biological materials → supramolecular systems durability Couple light harvesting part to a transducer cost and energy requirement Select part of spectrum where it will work (tunable)	Collaborative funding People Exchange of ideas Trained students and postdocs Sandpit? Interdisciplinary funding…….	NOW!

BALLOT BOX	17 dots

3. Theme: Charge Transfer Units with Long Lived Charge Separated States Allowing for Efficient Coupling to Catalytic Sites

UK Capability	Research Challenges	Involvement needed	Timescale
Expertise in many areas: synthesis, nanomaterials, biochemistry, characterisation but it is not joined up - need better collaborations. Need: better integration, ultrafast spectroscopies/facilities Strong:	Ultrafast spectroscopy → Understanding surfaces/interfaces in 'real life' situations - - →	 Sandpit	10 years 20+ years
	Better collaborations/integration as lots of expertise in disparate departments but not enough cross talk	Cross-disciplinary funding across research councils EPSRC/BBSRC/STFC	1-2 years
Overseas capability UK links Chergui, EPFL Lausanne Hanmarstrom, Sweden USA (Wasielewski, Brook Haven Nat Lab, Noyke DAMe Nat Lab)	Fundamental understanding of basic processes - NB process of charge separation; basic building blocks; surfaces; modelling of surface reactions Need better spectroscopies	Help with matching biologists/chemists/physicists 'Speed dating' to meet partners	Continuous and depends on above

Combine Themes 3 and 4
And Antennas

BALLOT BOX	24 dots

This is a cross-boundary topic/approach which can deliver

OTHER THEMES

12. Theme 12: Integration of Components "Smart" Matrices

UK Capability	**Research Challenges**	**Involvement needed**	**Timescale (years)**
Good in supramolecular assembly and surface-nanoscience Moderate in synthetic membrane science Good computational (all scale) modelling	1. Taking self-assembly from molecular/nano-scale to macroscopic structures	**MORE EXPERTISE IN GROUP!**	5
	2. Spatially specific functionalisation of synthetic membranes/transport specificity		10
Overseas capability UK links	3. Implementation of self-repair in nanoscale devices		20
Japan and US			
Collaborations in multi-scale modelling	4. Spatially specific, nanostructured electrode development		5
Combine with antennas	5. Multi-scale, multi-phase computation simulation from nm to cm	Again - NOT a real theme - simply a component of other approaches - combine	2
	6. Dynamic self-assembly of biological systems on surfaces		5

BALLOT BOX	10 dots

4. Theme: Multi-Electron Catalysis

UK Capability	**Research Challenges**	**Involvement needed**	**Timescale**
Patchy Vulnerable This area could be merged with "Photoelectrochem Fuel Production" **Overseas capability UK links** Sweden USA Germany Netherlands Japan	Dioxygen formation (water splitting) Carbon reduction Link photons to catalysis (robustness) Integration into functional device 'Smart' systems Electronic addressing	Biologists Photochemists Theoreticians Electrochemists Materials scientists Complex fluid	10 years to lab scale ↓? This seems the key issue vis - band gap too small for °OH → O_2

This is not a separate theme - it should be part of an overall strategy for artificial photosynthesis/water splitting.

BALLOT BOX	19 dots

13. **Theme 13: Solar Hydrogen Tower - Thermolysis of Water**

UK Capability	**Research Challenges**	**Involvement needed**	**Timescale**
Significant expertise on smaller-scale systems Academic and industrial expertise on catalysis Diffuse light concentrators	Insufficient sunshine and space Chemical challenges - using heat energy collected - thermolysis of water Engineering challenges - efficient integration of parts. Durability of materials Separation of H_2 and O_2 at high temperature Catalysis Methanol production (and other small molecules)	Probably not relevant for use in UK Funding for catalysis Engineering problems not the main challenges Surface scientists and chemical engineers communicating Funding for concentration of diffuse light	Proof of principle in 5 years?
Overseas capability UK links China (solar heating)			

NB: THOSE PRESENT HAVE LITTLE COLLECTIVE EXPERTISE ON SOLAR HYDROGEN TOWERS AND CATALYSIS - WE CAN'T GIVE VERY GOOD ANSWERS

BALLOT BOX	0 dots

……… Not a separate theme!!

Theme 15: Modelling of bioinspired nanodevices

UK Capability	**Research Challenges**	**Involvement needed**	**Timescale**
→ Strong in all individual components → CC a UK strength **Overseas capability UK links** → US strong → Germany strong	State of the art modelling key to underpin all other themes • Structure? • Mechanism? → know what we have got before moving on • In silico design → "very" long-term target with no clear path at present	→ People skilled → Collaborative Bring together experts and model and structure	NA This is not a theme as such. It is a vital part of virtually all main themes therefore subsume into those Should be generic to Themes 1-14 - AGREE - AGREE! The top-down approach described in the ESF report seems unrealistic - we can't design a "machine" until we understand how the bits work! This is the major role of theory, at least in the short (5 year?) timeframe - to shed light (!) on the component parts!

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BIOLOGICAL FUEL PRODUCTION

Bioreactors and higher plants
→ Nutrient input
Light
Siting/design
H_2
Carbon based

Biologists/chem. Eng need to work on the best system to use

Most appropriate bio-system to use

Genetic manipulation of plants and algae to improve photosynth efficiency

Associated problem of H_2 storage

Carbon - need to increase biomass, then engineer to produce value added chemicals
→ bioprocessing - Pharma
- Biofuels - long to short chain carbon - catalysis

H_2 simpler - Hydrogenase } enzymes
Nitrogenase }

CO_2 more complex, both input and products

Lots of UK skills in this area - requires focus

10-15 year H_2/CO_2 - longer

DISCUSSION

H_2 more challenging on metabolic work than CO_2

Trick is to produce C-chain of the right length to get best efficiency will take much more than 10 years

% efficiency's 100t h^{-1-Y} water, sugar 70t photosynthesis ~ 1% poss 5% under lab conditions theoretically as high as 10% if e^- comes from H_2O

Direct H_2 production rationale is to get better energy density

Cost unknown ie energy in vs energy out

CO_2 used as input - poss sequestration

Algae, will grow in areas unsuitable for land plants/food crops → large scale ocean plants - need for good control

No best strategy known

Economic studies - 10-15 year old → some studies in US, DOE studies

Currently an Australian patent for H_2 production from algae

Open system microbiology is unknown

Application of current methodologies - previous work now dated

Other bacterial means of fuel production

Use of marginal land/water; biomass based on land

These strategies do not impact on land used for food production

Environmental impact studies, none known + public perception

Use of waste water - potential for very clear way of treating sewage etc

Direct production of transport fuels
→ direct biodiesel production as well as ethanol
→ solid supports

PHOTOELECTROCHMICAL FUEL PRODUCTION

Lab max efficiency 10% - not yet practical in reality

- High T

For PV, getting close to thermodynamic limit

DSC using H_2O need a large free energy gradient

Light absorption and transport distances carriers nm<10 rather than μ therefore nanostructuring

Then need multielectron transfer → bio-mimetic (plants already do it)

Kinetic and O_2 evolution is still not clearly known

Molecular assemblies that do more than one thing absorption/separation e-generation catalytic centre built in

Also look at Cl^- production
→ H_2O_2
→ CO_2? Reduction of this is a key aim

Mechanisms and kinetics with studies at molecular level
→ computational modelling

Network - required to form a wider community must be inclusive, draw in wider funding and research road maps

Molecular oxidation catalysts, not very efficient
→ chemical programme of bio mimicking

$1e^-$ photochemistry to multi e^- multi proton catalysis
→ stability issues

Reactor engineering work needs to be done

Hydrogen solar - a C^o in UK working in this area

DISCUSSION

Q Scale up challenges - A Cost, low cost materials and substrates

Also separation tech, membranes

H_2 purity, purification processes

- Applicability to transport

- Use of Ruthenium, expensive element, market will drive

→ Mn is candidate and not much research is done
→ bio-mimetic, Mn used in nature (multiple Ox status)

- Currently internationally competitive

Q Any place for High T photocatalytic reactions water splitting - not very convenient
→ needs a dialogue with reactor engineers

- Ability of a system to work at pressure in an important Q

- Catalysis of e^- transfer at a surface

PRIMARY STEPS/SELF ASSEMBLY

- Photon harvesting and change separation

- Understanding biology

- Self assembled systems, bio-mimicry, self repair mechanisms

- KT with PV on methodologies etc

- Ability of bio-mimicry is limited → hard to reproduce, may be piecemeal

- Biochem, surface science etc

- Networking } to bring disciplines together
- Summer Schools }

- Much expertise in the UK - need to bring together and bring others in

- Id small parts that can be tackled

- Have to push bio-mimicry to achieve what is currently not achievable

- Look at molecular siting for most efficient operation

- Fundamentals to be worked out for bio-mimicry to produce robust molecules

DISCUSSION

- Now lots of new molecular info, that is moving this area forward

- Many current methods use very crude self assembly whereas biology produces some very complex structures

- Liquid crystal chemistry an area of interest in self assembly - non organic system

- Self assembly of multiple functional materials

GENERAL DISCUSSION POINTS

- This is one of <u>the</u> grand challenges
- Needs a long-term effort
- UK has <u>very good</u> capability in this area
- Discipline hopping award
- Needs X-cross Council activity
- Demonstrable milestones
- Road mapping exercise [e.g. H_2 economy from DOE]
- Capacity? - young researchers activity targeted at the next generation (eg materials research soc]

- Training an aspect of the Network
- Energy fellowships