

# Delft Research Centre for Sustainable Energy

*"SUSTAINABLE ENERGY, EXTRACTION,  
CONVERSION AND USE; SENEUCU"*

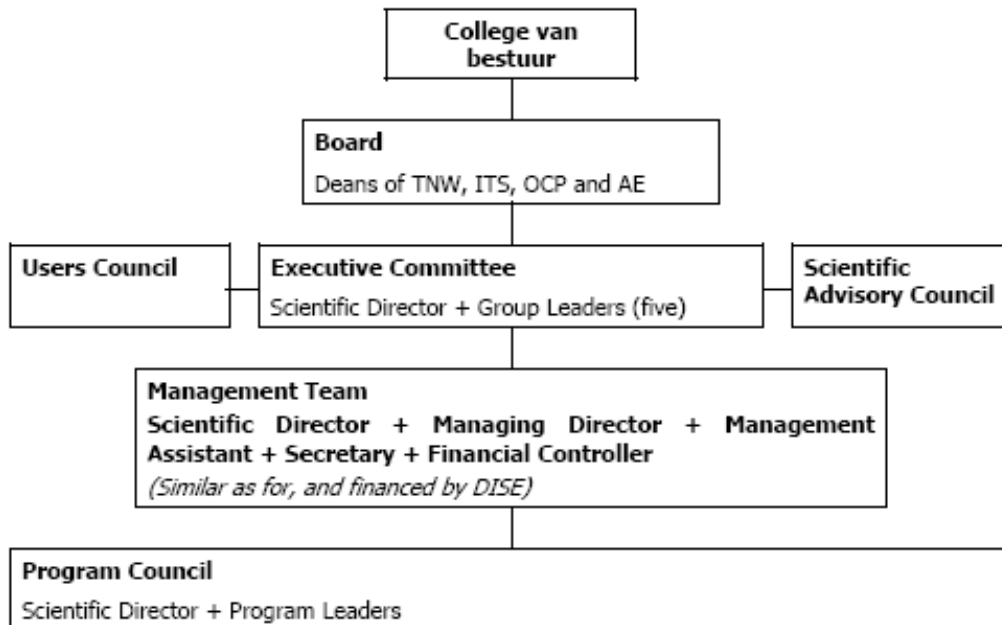
**ANNUAL REPORT  
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## 1. General Information

The management structure of this DRC is depicted in the following diagram along with the members of the various groups.



1. **College van Bestuur (CVB):** Ir. G.J. van Luijk (President), Prof. Dr. Ir. J.T. Fokkema (Rector magnificus), Drs. P.M.M. Rullmann (Member)
2. **Board:** Prof. Ir. K.Ch.A.M. Luyben (Chairman), Prof.Dr.Ir. J. van Katwijk, Prof.Drs. M. Waas, Prof. B.A.C. Droste.
3. **Scientific Director (SD):** Prof.Dr. J. Schoonman
4. **Executive Committee (ExCo):** Prof. Dr. J. Schoonman, Prof. Dr. S.J. Picken, Prof. Dr. J. Moulijn, Prof. I. L. van der Sluis,
5. **Management Team (MT):** Prof. J. Schoonman (SD), Dr. E.M. Kelder (Managing Director), Mrs. A.M.C. Barrow (Management Assistant), Mrs. M.A. de Bruijn (Secretary), Mrs. J.A.M. van Vugt (Financial Controller).
6. **Program Council (ProC):** See Chapter 4: personnel.
7. **Users Council (UseCo):** Dr. G.H.M. Calis, Ir. M.R. van Groeningen, Dr.Ir. M.J.G. Jak, Dr. H.P.C.E. Kuipers, Dr. L.B.J. Vertegaal, Dr. E.M. Witte. (Co-ordinates see Attachment I)
8. **Scientific Advisory Council (SAC):** Prof.Dr. M. Grätzel, Prof.Dr.Ir. P.J. Jansens, Prof.Dr.Ir. G. Ooms, Prof.Dr. F.B. Prinz, Prof.Dr. F.W. Saris, Prof.Dr. W. Sinke, Prof.Ir. L. van der Sluis, Prof.Dr.Ir. W.P.M. van Swaaij, Prof.Dr.Ir. M.P.C. Weijnen. Prof.Dr.Ir. S. van der Zwaag, Prof. Dr. J-M Tarascon. (Co-ordinates see attachment I).

## 9. 2. Scientific background, goals and progress

### 2.1 Introduction and goals

Tackling the fundamental and focused applied research issues which is a prerequisite to contributing to paving the way for a future more sustainable energy supply.

The scientific program addresses fundamental and applied key questions concerning efficient and cheap conversion of solar and small scale wind energy into electrical energy, its storage and utilization in society. In addition, the program addresses fundamental and applied key questions concerning a Hydrogen Economy. The efficient and economic production and safe storage of hydrogen using renewable energy sources is being studied. The introduction of a hydrogen economy and its social acceptance will heavily rely on the safe storage and societal acceptance. Therefore, along with a substantial research effort on the production of sustainable hydrogen, the safe and cheap storage of hydrogen comprises an important part of the scientific program with implicit attention to societal aspects. For the conversion of hydrogen into electrical energy, fuel cells are the choice. The concept of exergy will be used to define sustainability in its technological context.

The scientific program focuses on innovative design, production, storage, and application of (nanostructured) materials for advanced devices for the utilization of sustainable energy, in particular, solar and wind energy. Electricity production with photovoltaics (PV) and wind energy does not coincide with the demand profile. Off-grid electrical energy must be stored. Lithium-ion battery technology and hydrogen storage will offer opportunities for decentralized PV and wind applications. Biomass gasification and purification, as well as novel hydrogen storage concepts in organic liquids, are to be related to innovative fuel cell designs, while novel storage concepts of hydrogen are directed to absorption in nanostructured light-weight materials based on magnesium-alloy, or sodium and lithium alanates. In the program the pathways of "Molecule to Process" and "Molecule to Product" shall be fully explored via intensive collaborations between the projects in the two main streams "Electrons" and "Protons".

The scientific program will include advanced theoretical modelling and advanced characterization techniques, in several instances, uniquely available at TUDelft. The program will be financially supported by the TUDelft from 2003 till the end of 2009. At mid-term in 2006, go/no-go decisions will take place for the projects in the program. In case projects are not successfully evaluated, they may be terminated. Evaluation criteria are listed as indicators in the description of work (DoW) by project – these indicators then are the basis for the evaluation for each project. The DoW contains the technical and scientific paragraph by project, while the implementation into SENECU will be the collective responsibility of the participants. In order to carry out a program of this size, a few million Euros per year is required. The TUDelft contribution to SENECU will be 308, 727, 727, and 727 kEuros for the years 2003, 2004, 2005, and 2006, respectively. It is stressed by the TUDelft governing board, that the financial support needs to be seen and used as seed money, so as to stimulate and promote the development of a durable and fruitful collaboration and to strengthen excellence on sustainable energy by bringing together the critical mass of resources and expertises needed to provide National leadership and be a world acknowledged force on that topic. The expertise will be networked around a program of activities (PA) aimed at creating a durable collaboration of the research capacities of the SENECU participants while, at the same time, advancing knowledge on the topic. The program activities defined are:

- Shared Program Activities;
- Program of Executed Research;
- Activities on Dissemination;
- Management Activities;

## 2.2 Progress and Highlights

### *Shared Program Activities*

The shared program activities are described basically within the defined clusters, these are: Solar, Biomass, e-Storage, H-Storage, and Utilization. A new cluster "Ionic Liquids" has recently been defined and accepted. This cluster was created as many other clusters may use ionic liquids in the future. Hence, in order to avoid spreading thin of the subject over the clusters, we believe this new cluster was necessary.

Furthermore, with respect to various synthesis methods for nanomaterials, a close collaboration has been formed between the DCT groups of AC and PART, covering at least a quarter of the projects.

A similar process has started on sharing characterisation equipment, however, formal agreements have not been achieved yet.

With respect to shared projects, a crosslink between various projects was established in the e-Storage cluster. Here the participants may use the infrastructure of the new European Network of Excellence "Alistore", which is focussed on materials for rechargeable Li-ion batteries.

Another externally funded project, financed by NWO-ACTS, bridges the clusters Solar and H-Storage.

Within the Solar cluster, optical diagnostic equipment is being shared, in particular the Raman spectrometer of AC was often used in that respect.

### *Program of Executed Research*

#### *Cluster 1: Solar*

Two automatic spray deposition set-ups were constructed and are in full operation. The possible presence of sub-bandgap electronic states in  $\text{CuInS}_2$  was investigated with the Kelvin probe technique, but without success. A detailed time-of-flight study was undertaken to measure the mobility of the charge carriers in nanostructured electrodes. This study has provided new information about the charge-transport mechanism in solar cells comprising nanocomposites of  $\text{TiO}_2$  and  $\text{CuInS}_2$ .

Neutron scattering and modeling work on discotic materials show that the picosecond dynamics is characterised by sliding and concertina motions of the disks, and that rotational relaxation is in the 100 nanosecond region, which is strikingly similar to the fluorescence decay measurements, suggesting coupling between the disk-rotation and exciton relaxation. Surprisingly, high frequency C-C stretches and CCC deformations in the  $\sim 30$  femtosecond timescale also cause large changes in charge transfer between two disks. A whole new range of phase behavior and dynamics has been found for discotics in which one of the 6 tails has a different length.

Dynamics of oligoethyophenes and polythiophene have been studied in the femtosecond to 100 picosecond timescale. This enables us to establish the time-averaged distribution of conformations and also how conformations evolve with time. From this we can establish which nuclear degrees of freedom are important in electron-phonon coupling and charge transfer processes. We now have data on the detailed dynamics of discotics and conducting polymers. A complex between a discotic and charge transfer compound, TNF, is particularly important because it has record high electron mobility of  $5 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ .

Silicon films have been deposited with RF-PECVD using hydrogen diluted silane, to obtain protocrystalline silicon films, which are interesting because of their increased stability compared to standard amorphous silicon films. From the electrical and optical measurements it was found that layers deposited at a rate equal to the rate obtained with standard amorphous thin films are not as stable as required. In order to optimize the deposition for higher stability layers, a series of samples using different deposition conditions has been prepared. In parallel with the electro-optical characterization, the structural properties of the layers grown from  $\text{H}_2$  diluted silane was analyzed.  $1 \mu\text{m}$  thick samples were prepared on different substrates and analysed via High Resolution Electron Microscopy. We identified the transition between the amorphous and microcrystalline phase and thus the conditions for

protocrystalline growth. Results from Raman spectroscopy carried out at the Laboratory of Inorganic Chemistry on the same samples show a corresponding trend.

The influence of substituents on the structure of spin-coated meso-tetraphenylporphyrin thin films has been characterized using UV/VIS, steady-state and time-resolved fluorescence spectroscopy, for unsubstituted meso-tetraphenylporphyrin (TPP) and for meso-tetra(4-ethylphenyl)porphyrin (TEPP). The efficiency of charge carrier photogeneration in these films in TiO<sub>2</sub>/porphyrin bilayer systems has been determined using the Time-Resolved Microwave Conductivity (TRMC) technique. We deduced that TPP molecules tend to form face-to-face dimers or larger aggregates, which strongly suppresses fluorescence, decreases the exciton lifetime, and enhances radiationless decay of excitons. In contrast, TEPP molecules do not exhibit aggregation, resulting in a ca. 20 times higher fluorescence yield, an enhancement of the exciton lifetime from 260 ps to 800 ps, as well as a higher fluorescence rate constant. Since excitons in thin films of these porphyrin derivatives mainly diffuse by Förster energy transfer, the higher fluorescence rate in TEPP antenna layers results in an enhancement of the exciton diffusion coefficient from  $2 \cdot 10^{-9}$  m<sup>2</sup>/s to  $7 \cdot 10^{-8}$  m<sup>2</sup>/s. Together with the longer exciton lifetime, this enlarges the exciton diffusion length from 7 Å to 75 Å. For porphyrin/TiO<sub>2</sub> bilayers, this results in an increase of the charge separation efficiency per incident photon at the Soret band maximum from 1.2 % for TPP to 6.2 % for TEPP.

#### **Cluster 2: Biomass**

An evaluation of five different gasification processes for the production of a hydrogen-rich synthesis gas was performed. The CFD modelling of a Solid Oxide Fuel Cell (SOFC) stack (corp. ECN) has started recently dealing with the "Development of a micro combined heat and power system based on low/high temperature polymer fuel cell's" (corp. ECN). " Small hydrogen refuelling stations" (corp. GM-Germany), and "Development of a SOFC-GT" (Gas Turbine) hybrid system.

The project Early Agglomeration Recognition System I was successfully finished in 2004. The earlier developed method for detection of agglomeration in bubbling fluidized beds (the so-called attractor comparison method) has been adapted for the use in circulating fluidized beds (CFBs) and has been tested in our lab-scale CFB. In cooperation with the control software company IPCOS, the method has been implemented in a robust, industrial software package. It is currently being tested in a pilot-scale installation at Chalmers University (Sweden); full-scale tests in the CFB gasifier of Essent at the Geertruidenberg power plant are scheduled for 2005. At the same time, we continue to carry out more fundamental work to increase insight into the agglomeration phenomena and to improve the applied to signal analysis methods (better sensitivity and selectivity).

#### **Cluster 3: e-Storage**

The work for the Network of Excellence "Alistore" has been implemented in this part of the research and vice versa. To date, analyses can be performed with all available techniques one can practically think of – these include, for instance: SEM, TEM, HREM, XRD, ND, EXAFS, NMR, Mössbauer spectroscopy. The TUDelft has created a platform for Electron Microscopy with an other Alistore partner in that respect.

Electrostatic Spray Pyrolysis has been re-activated to form nanopositives oxides – the set-up was made in close collaboration with Prof. Schmidt-Ott/Dr. Marijnissen. Spark Discharge generation has been done to synthesise nanopowders of Mg<sub>2</sub>Si – the research was done in close collaboration with Prof. Schmidt-Ott. Improvements of metal current collector surface kinetics has been found using SiC nanoparticles.

Magnetic Pulse Compaction has been applied to various metallic powders and alloys for making "rods", required for the Spark Discharge Generation.

The comparison of bulk and nanopowder TiO<sub>2</sub> electrode materials yields unexpected, but highly interesting results, i.e. large changes in the Li site occupations and ionic dynamics in the nanostructured compounds compared to the bulk. The interplay between electronic

and ionic degrees of freedom is observed in both bulk and nanostructured materials. Concerning cross-boundary ionic diffusion, within milliseconds all Li ions exchange between Li-rich and Li-poor phases in the solid electrode material based on Li intercalated  $\text{Li}_4\text{Ti}_5\text{O}_{12}$ . First trial experiments show that for a nanostructured electrode-electrolyte composite there is full exchange of Li ions between the solid and the liquid on seconds timescales. The diffusion of large cations like Mn and Ni was observed during the intercalation of Li in  $\text{Li}[\text{Mn},\text{Ni}]_2\text{O}_4$  using neutron diffraction. The ionic conduction of the lithium electrolyte made by blending PEO with inorganic nanoparticles is enhanced significantly. This enhancement was shown to be due to interface effects and not to enhanced polymer dynamics.

#### **Cluster 4: $\text{H}_2$ -storage**

It has been established that hydrogen ( $\text{H}_2$ ) can be stabilised in certain water clathrates at high pressure. Our research showed that the use of promoter molecules reduces the pressure from 2300 to 100 bar. The family of tectosilicates known as clathrasils presents the same topology as the water clathrates. It is expected that hydrogen can be accommodated in some clathrasil structures as well, most likely at standard pressure.

As a proof of principle for hydrogen storage in clathrasils, it was decided to synthesise a framework in which  $\text{H}_2$  molecules could be trapped. Theoretical calculations on zeolites - which are related materials to clathrasils - showed that hydrogen can diffuse through the 6-rings of a sodalite cage, but not through 5-rings. A number of clathrasil structures contain cages uniquely composed of 5-rings: the synthesis of these structures in the presence of  $\text{H}_2$  should lead to the trapping of hydrogen molecules inside the 5-ring cages.

Different clathrasils were prepared both under  $\text{H}_2$  and  $\text{N}_2$  atmosphere, in order to determine whether  $\text{H}_2$  could be trapped inside the cages and in which amounts, and whether its presence would direct the synthesis towards a specific structure. Characterisation of the synthesised materials in order to study the presence of  $\text{H}_2$  or  $\text{N}_2$  inside the clathrasil cages is in progress (Solid-state NMR, Temperature Programmed Desorption).

To initiate the hydrogenation of naphthalene, a temperature of over  $200^\circ\text{C}$  is needed, and primary experiments indicated that hydrogenation is rather difficult. Styrene is also a good candidate to store sufficient hydrogen, and easier to hydrogenate, as was determined using ATR-FTIR as analytical tool, showing 100% conversion at  $120^\circ\text{C}$  and 50 bar  $\text{H}_2$ . The main products are ethyl-cyclohexane ( $\text{C}_8\text{H}_{16}$ , ca. 87 %) and ethyl-benzene ( $\text{C}_8\text{H}_{10}$ , ca. 12 mol%). The total hydrogen storage density is about 6.5 wt%. A series of experiments of hydrogenation of styrene at various concentrations, temperatures and pressures was carried out with the aim of optimizing the reaction conditions in order to obtain sufficient hydrogen storage density. An article will be prepared on this subject.

The storage of hydrogen in biological systems is being studied and the enzyme named *Pyrococcus furiosus* is available for hydrogen storage reactions, since this enzyme is active even at  $100^\circ\text{C}$ , while most other enzymes are active at much lower temperature. The first organic substrate used is 3-methoxy benzoic acid, however, the aromatic ring is too difficult to be hydrogenated by this enzyme at low  $\text{H}_2$  pressures. Since pyridine rings can be hydrogenated easier than aromatic rings, the nitrogen hetero-aromatics may be suitable substrates for this application. Further investigations on these compounds will be carried out within this project.

Nanoparticle production methods that are flexible with respect to the particle composition and size are being developed. The current approaches include electrospray, non-equilibrium plasma and spark ablation. 10 nm Palladium nanoparticles as a hydride forming species have been produced by the latter method as a first step. A beam of such particles in inert gas has been focussed to a substrate and the particles successfully bridged electrodes. This principle will be applied to sensitive hydrogen sensing. Progress has been made in achieving the required gas purity for non-oxidizing production of metal particles. The scaling up of electrospray is being pursued in connection with the newly acquired project EWICON on electrostatic wind energy conversion.

**Cluster 5: Utilization**

Laboratory system components for the electrical circuitry used as interfaces between the energy sources and energy consumers were tested separately. The implementation of the system components were finally done successfully. The control system is currently being programmed to operate the laboratory autonomously.

Comparison of processes for production of Hydrogen by thermochemical reactions and hot electrolysis. Assessment of numerical codes for the core design of Very High-Temperature Reactors (VHTR) (cooperation with Georgia-Tech, US). Contribution to the validation of numerical codes for the design of the Next Generation Nuclear Plant (cooperation with INEEL, Idaho, US). Design of a Gas-cooled Fast Reactor (GFR) core with recycling of plutonium and minor actinides. Design and safety assessment of the Experimental Test Demonstration Reactor (cooperation with CEA, France)

A method has been developed to more properly determine the work potential of (biochemical) compounds in intracellular solutions. The method has been used to analyze some well-known biochemical processes step by step, and remarkably high thermodynamic efficiencies have been revealed in this way. The method has been tested and perfected to account for all relevant thermodynamical effects, and also the thermodynamic analyses of the metabolic processes have been substantiated and are now largely completed. Publications of the method and mentioned applications will follow shortly. Also, additional work on thermodynamic inefficiencies and sustainability was presented at the annual meeting of the American Institute of Chemical Engineers (AIChE) in Austin, USA, and successful collaboration was achieved with the Ceramic Membrane Centre "The Pore" within the framework of the Delft Research Centres.

Main highlights with respect to wind energy are the development of a method for qualification of combinations of wind turbines and buildings, the assessment of the aerodynamic performance of VAWT wind turbine operation in the flow over buildings, the further development of Turby, a VAWT wind turbine, for application on rooftops together with Core International, a Dutch based Company, and participation in a qualification document for the Urban wind power project on the Freedom Tower New York, USA.

**2.3 Users Council's Report**

N/A

## 2.4 Research Output

Since an important goal in this Delft Research Centre is integration and use of mutual infrastructure and knowledge, only shared publications are listed here. Publications from individual groups associated with the topics of SENECU are gathered in Attachment II. The invited lectures are listed without this distinction.

### Refereed papers

1. Dicker, G., M.P. de Haas, J. M. Warman, D.M. de Leeuw, L.D.A. Siebbeles, The disperse charge-carrier kinetics in regioregular poly(3-hexylthiophene). *Journal of Physical Chemistry B*, 108 (2004) 17818-17824
2. Eijck, L. van, K. Senthikumar, L.D.A. Siebbeles, G.J. Kearley, A quantitative study of the charge-transfer between conjugated thiophene rings in vibrationally excited states. *Physica B*, 350 (2004) 220-223
3. Eijck L. van, A.S. Best, G.J. Kearley, Effect of nanocrystalline materials on ionic interactions in polymer electrolytes. *Macromolecules* 37 (2004) 9591-9595
4. Florusse, L.J., C.J. Peters, J. Schoonman, K.C. Hester, C.A. Koh, S.F. Dec, K.N. Marsh, & E.D. Sloan, Stable Low-Pressure Hydrogen Clusters Stored in a Binary Clathrate Hydrate. *Science* 306 (2004) 469-471
5. Fratiloiu, S., L.P. Candeias, F.C. Grozema, J. Wildeman, L.D.A. Siebbeles, VIS/NIR absorption spectra of positively charged oligo(phenylenevinylene)s and comparison with time-dependent density functional theory calculations. *Journal of Physical Chemistry B*, 108 (2004) 19967-19975
6. Grozema, F.C., P.Th. van Duijnen, L.D.A. Siebbeles, A. Goossens, S.W. de Leeuw, Electronic structure of thienylene vinylene oligomers: singlet excited states, triplet excited states, cations and dications. *Journal of Physical Chemistry B* 108 (2004) 16139-16146
7. Huang Foen Chung, R.W.J.M., & S.W. de Leeuw, Ionic conduction in LiI-alpha,gamma-alumina: a molecular dynamics study. *Solid State Ionics* 175 (2004) 851-855
8. Kearley, G.J., F.M. Mulder, S.J. Picken, P.H.J. Kouwer and J. Stride, Dynamics of discotic methoxy triphenylene molecules from quasielastic neutron scattering and molecular dynamics simulations. *Chemical Physics*, 292 (2003) 185-190
9. Kruglova, O., F.M. Mulder, S.J. Picken, & G.J. Kearley, Analysis of quasielastic neutron scattering (QENS) data of discotic systems using different molecular dynamics (MD) models. *Physica b*, 350 (2004) e1003-e1005
10. Landschoot, N. van, E.M. Kelder, P.J. Kooyman, C. Kwakernaak, & J. Schoonman, Electrochemical performance of Al<sub>2</sub>O<sub>3</sub>-coated Fe doped LiCoVO<sub>4</sub>. *Journal of Power Sources*, 138 (2004) 262-270
11. Mulder, F. M., J. Stride, S.J. Picken, P.H.J. Kouwer, M.P. de Haas, M.P., L.D.A. Siebbeles, G.J. Kearley, Dynamics of a Triphenylene Discotic Molecule, HAT6, in the Columnar and Isotropic Liquid Phases. *Am. Chem. Soc.* 125 (2003) 3860-3866
12. Smit, C., R.A.C.M.M. van Swaaij, H. Donker, A.M.H.N. Petit, W.M.M. Kessels, and M.C.M. van de Sanden, Determining the material structure of microcrystalline silicon from Raman spectra. *Journal of Applied Physics*, 94 (2003) 3582-3588
13. Wagemaker, M., F.G.B. Ooms, E.M. Kelder, J. Schoonman, G.J. Kearley, & F.M. Mulder, Extensive migration of Ni and Mn in lithiation of ordered LiMg<sub>0.1</sub>Ni<sub>0.4</sub>Mn<sub>1.5</sub>O<sub>4</sub> spinel. *Journal of the American Chemical Society* 126 (2004) 13526-13533
14. Wagemaker, M., D.R. Simon, E.M. Kelder, J. Schoonman, & F.M. Mulder, Proton positions in spinel H<sub>0.9</sub>Li<sub>0.1</sub>[Li<sub>0.33</sub>Ti<sub>1.67</sub>]O<sub>4</sub>, an ion-exchanged spinel Li<sub>1</sub>[Li<sub>0.33</sub>Ti<sub>1.67</sub>]O<sub>4</sub>. *Physica b*, 350 (2004) e995-e998
15. Wagemaker M., R. van de Krol, A.A. van Well, Nano-morphology of lithiated thin film TiO<sub>2</sub> anatase probed with in situ neutron reflectometry. *Phys. B*, 336 (2003) 124
16. Warman, J.M., M.P. de Haas, G. Dicker, F.C. Grozema, J. Piris, M.G. Debije, Charge Mobilities in Organic Semiconducting Materials Determined by Pulse-Radiolysis Time-Resolved Microwave Conductivity: pi-Bond-Conjugated Polymers versus pi-pi-Stacked Discotics. *Chemistry of Materials*, 16 (2004) 4600-4609
17. Zanden, B. van der, R. van de Krol, J. Schoonman, & A.P.L.M. Goossens, Enhanced photoluminescence at poly(3-octyl-thiophene)/TiO<sub>2</sub> interfaces. *Applied Physics Letters* 84 (2004) 2539-2541

### Invited lectures

1. Goossens, A.P.L.M., Nanocomposites between N-type and P-Type Semiconductors: Towards A New Generation of Solar Cells. Graubunden, Switzerland, August 2004, Nanoparticles from the Vapor Phase Synthesis with Chemical and Biochemical Applications
2. Goossens, A.P.L.M., Photovoltaic active nanocomposites of TiO<sub>2</sub> and CuInS<sub>2</sub>: structure and properties of a novel solar cell design. Stuttgart, Germany, September 2003, 9th European Conference on Solid State Chemistry
3. Goossens, A.P.L.M., Synthesis and characterization of nanocomposites of inorganic n- and p-type semiconductors: towards a new solar cells design. Leuven, Belgium, September 2003, Eleventh symposium on unconventional photoactive systems (EPS11)
4. Goossens, A., New generation solar cells: what to expect?, The Hague, The Netherlands, November 14 – 16, Munish 2003 Conference
5. Goossens, A., Nanocomposites between n-type and p-type semiconductors: towards a new generation of solar cells. Davos, Switzerland, August 8-13, 2004, Engineering Conference International (ECI) Nanoparticles from the vapor phase synthesis with chemical and biochemical applications.
6. Goossens, A., Nanocomposites of n-type and p-type semiconductors: towards a new generation of solar cells. University of Mar del Plata, Argentina, October 26 - November 6, 2004 visit to INTEMA
7. Kearley, G.J., Understanding the Dynamics of Stacked Discotic Molecules. Delft, 14 oktober 2003, Polymer Dynamics

## lectures series

8. Kelder, E.M., S.J. Picken, R.A. Sheldon, S.W. de Leeuw, C.J. Peters, G.J. Kearley, J.A. Moulijn, & J. Schoonman, Ionic Liquids. Delft, November 2004, Alistore/DISE Workshop
9. Kelder, E.M., Li-ion battery principle for sensor applications. Delft, January 2004, Second DISens symposium
10. Kelder, E.M., Migration on Mn and Ni upon lithiation of ordered LiMg delta Ni<sub>0.5-δ</sub>Mn<sub>1.5</sub>O<sub>4</sub> spinels. San Francisco, USA, April, 2004, MRS Spring Meeting
11. Krol, R. van de, C.S. Enache, & J. Schoonman, Nanostructured Metal Oxides; Promising (Photo)Catalysts for the Production and Storage of Hydrogen. Eindhoven, October 2004, ISIEEM 2004
12. Krol, R. van de, Metal Oxide Catalysts for Hydrogen Production. Eindhoven, November 2003, KNCV Symposium on the Electrochemistry of Hydrogen
13. Krol, R. van de, Transition Metal Oxide Catalysts for the Production and Storage of Hydrogen - Better Catalysts through Defect Chemistry. Vrije Universiteit Amsterdam, October 2003, Colloquium Condensed Matter Physics group
14. Manea, F., J. Schoonman, & C. Radovan, Electrochemical Sensors for Environmental Monitoring. Brasov, Roemenie, Juni 2004, First International Conference on ENvironmental EDucation (EnvEdu 2004)
15. Marijnissen, J.C.M., Electro Hydrodynamic Atomization and its Applications. Budapest, September 2004, European Aerosol Conference 2004
16. Mulder, F.M., Neutrons and numerical methods for energy storage and conversion materials. Grenoble, 2004, Neutrons and Numerical Methods N<sub>2</sub>M<sub>2</sub>
17. Mulder, F.M., Ions and molecules in motion in batteries and solar cells. Arcachon, 2004, 7<sup>th</sup> International Conference on Quasielastic Neutron Scattering QENS2004
18. Mulder, F.M., et al., The life and times of a Li ion in TiO<sub>2</sub> battery anode materials. Bordeaux, 2003, Lithium Battery Discussions
19. Kearley, G.J., Neutrons, vibrations and simulations. Department of Energy (USA) Washington 2004, Neutrons in Chemical Research
20. Nanu, M., J. Schoonman, & A. Goossens, Inorganic nanocomposites of n- and p-type semiconductors: a new generation of 3D solar cells. Helsinki, Finland, August 16-18, 2004, ALD2004 Conference
21. Ommen, J.R. van, Monitoring Multiphase Flows using Attractor Comparison. Båstad, Sweden, October 20-21, 2004, Fifth Programme Conference on Multiphase Flow
22. Prins, P., Fast charge transport along isolated molecular wires of thienylene-vinylene. Cornell University, State of New York, US, 14-18 juni 2004, Sixth International Symposium on Functional pi-Electron systems
23. Savenije, T.J., The Mobility and Decay Kinetics of Charge Carriers in Bulk Heterojunctions. Bad Gastein, Salzburg, Österreich, 14-20 maart 2004. 16th Workshop on Quantum Solar Energy Conversion - (QUANTSOL 2004)
24. Savenije, T.J., Singlet and triplet exciton diffusion and interfacial charge separation in porphyrin/TiO<sub>2</sub> double-layers. Paris, France, 4-9 juli 2004, IPS-15, Fifteenth International Conference on Photochemical Conversion and Storage of Solar Energy
25. Schimmel H.G., et al., Hydrogen dynamics in magnesium metal (alpha phase) observed using neutron scattering and simulations. Krakow, Poland, 2004, Metal Hydrides
26. Siebbeles, L.D.A., Dynamics of charge carriers and excitons in organic materials for opto-electronic applications. South Hadley, MA, USA, 25-30 juli 2004, Gordon Research Conference on Electronic Processes in Organic Materials, Mount Holyoke College
27. Siebbeles, L.D.A., Dynamics of charge carriers and excitons in organic materials for opto-electronic applications. Waterville, ME, USA, 20-25 juni 2004, Gordon Research Conference on Radiation Chemistry, Colby College
28. Siebbeles, L.D.A., A new ultrashort laser/electron pulse facility for the study of charge and exciton dynamics in functional materials. Brookhaven Nat. Lab. USA, 26-28 juni 2004, International Symposium on ultrafast accelerators for pulse radiolysis
29. Siebbeles, L.D.A., Exciton diffusion and charge separation in porphyrin/TiO<sub>2</sub> belayers, Global Climate and Energy Project. Stanford University, U.S.A., 18-19 Oktober 2004, Workshop on Solar Energy
30. Schoonman, J., R. van de Krol, E.M. Kelder, & A.P.L.M. Goossens, Designing a new generation of solar cells and rechargeable batteries based on mesoscopic architectures. MIT Cambridge MA, USA, August 2003, ICE 2003 Conference
31. Schoonman, J., Impedance spectroscopy of materials for energy conversion and storage systems. Warszawa, Poland, September 2003, International Workshop Impedance Spectroscopy for Characterisation of Materials and Structures (IMSPEMAS)
32. Schoonman, J., M. Nanu, J. van Landschoot, R. van de Krol, & A.P.L.M. Goossens, Nano-structured materials for conversion and storage of renewable energy. Moscow, June, 2004, MSU-HTSC VII
33. Schoonman, J., M. Nanu, A.P.L.M. Goossens, S.A. Zavyalov, & A.N. Pivkina, Nanostructured Materials for Conversion and Storage of Solar Energy. San Francisco, USA, April 2004, MRS Spring Meeting
34. Schoonman, J., Duurzame Energie: een Zonnige Toekomst. Sociëteit De Witte, Den Haag, October 2003 Utrechtse Alumni
35. Schoonman, J., Nanostructured Electroceramics for Conversion and Storage of Sustainable Energy. Yokhoma, Japan, October 2003, 6th International Conference: ECOMATERIALS, Joint Workshop: Ecomaterials & Recycling
36. Schoonman, J., Nanostructured functional materials for energy conversion and storage systems. Trieste, Italy, December 2003, EuroNanoForum 2003
37. Schoonman, J., Nanostructured Functional Materials. Sozopol, Bulgaria, September 2004, NATO Advanced Study Institute, Nanostructured and Advanced Materials for Applications in Sensor, Optoelectronic and Photovoltaic Technology
38. Schoonman, J., Innovations in Energy Storage. Ambassadors Residence. Washington DC, April 2004, Symposium "Sustainable Energy: the Dutch Perspective"

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40. Schoonman, J., Composite Nano-Structured Lithium Battery Materials. Munster, Germany, October 2004, 84th International Bunsen Discussion Meeting: Structure and Dynamics of Disordered Materials
41. Schoonman, J., The (defect)chemistries for nanostructured materials for 3D solar cells, rechargeable lithium-ion batteries, and hydrogen storage. St. Andrews, UK, October 2004, Irvine Review 2004
42. Schoonman, J., In Pursuit of the Future. Brasov, Romania, November 2004, Meeting Transilvania University
43. Schoonman, J., Nanostructured materials for conversion and storage of sustainable energy. Rome, Italy, November 2004, Present Situation and Forecasts of Nanotechnology in: Materials, Health and Medical Systems, Energy
44. Schoonman, J., Nanostructured Funtional Materials. Kyoto, Japan, December 2004, 9th Seminar on Hydrogen Energy
45. Schoonman, J., Sustainable Energy Resarch in the European Union. Kyoto, Japan, December 2004, The 2nd International Symposium on Sustainable Energy System
46. Wagemaker, M., et al., Li intercalation in TiO<sub>2</sub> battery anode materials. Monterey CA, USA, 2003, Solid State Ionics-14
47. Warman, J.M., Anisotropy in the mobility and photogeneration efficiency of charge carriers in aligned films of discotic hexabenzocoronenes studied by FP-TRMC. Strasbourg, France, 25 mei 2004, E-MRS 2004 Spring meeting of the european materials research society
48. Warman, J.M., Exciton diffusion and interfacial charge separation in antenna-coated layers of TiO<sub>2</sub> studied by FP-TRMC. Golden Colorado, USA, 7 mei 2004, National Renewable Energy Laboratory
49. Warman, J.M., Exciton diffusion and interfacial charge separation in semiconductor/antenna bilayers studied by FP-TRMC. San Antonio, TX, USA, 11 mei 2004, The 205th meeting of The Electrochemical Society

### Theses

1. Piris, J., Optoelectronic Properties of Discotic Materials for Device Applications, PhD Thesis, TU Delft 2004, ISBN 90-407-2520-9
2. Kroeze, J.E., Photoinduced Charge Separation in Dye-Sensitized Films of Smooth and Nanocrystalline TiO<sub>2</sub>, PhD Thesis, TU Delft 2004, ISBN 90-407-2522-5
3. Dicker, G., Photogeneration and dynamics of charge carriers in the conjugated polymer poly(3-hexylthiophene), PhD Thesis, TU Delft 2004, ISBN 90-407-2542-X

### Book Editorship

- 1 Kelder, E.M., E.R. Leite, J.M. Tarascon, & Y.M. Chiang, (Eds.). Nanostructured Materials in Alternative Energy Devices. Warrendale, Pennsylvania, USA(2004) MRS

### Summary

#### Overview of the main research output

	2003-2004
Refereed shared papers	17
Refereed individual group papers	79
Invited lectures	49
Theses	3
Book editorships	1

### 3. SENEUCU's policy evaluation

The progress of this DRC will be evaluated at the end of 2006. Therefore, certain verifiable targets have been defined, which become opportune at the end of 2006. These targets are given in Attachment III. This part further provides information on the non-scientific results obtained so far, and is seen as a prerequisite for a proper operation of this DRC.

#### 3.1 Public image and communication

##### Overview of general information delivery to the public

Dates	Type	Type of audience	Countries addressed	Size of audience
24/06/04	Media briefing, University magazine "TUDelta", 21 (36, 2004) 7 "Nanopoeder als geest in de fles" <a href="http://www.delta.tudelft.nl/archief/j36/n21/18717">www.delta.tudelft.nl/archief/j36/n21/18717</a>	General public TUDelft audience+	NL	10.000
23-24/ 11/04	Combined Workshop of SENEUCU and ALISTORE in Delft	R&D, S&T	All	100
06/11/04	Technologiedag 2004; Leven met Risico's	Public	NL	350

##### Newspapers and public information

- Kooyman, PJ (18-12-2004). Bedekking van nanodeeltjes is nog niet volledig. NRC Handelsblad.
- Krol, R van de, & Luzzi, A (2004). Report on the kick-off meeting of the IEA/Annex 20 programme "Hydrogen from waterphotolysis", TUD.
- Kooyman, PJ, & Schoonman, J (2004, February ). Titanium dioxide nanoparticles in sunscreen cream. Theater Concordia, Den Haag, Workshop "Kansen en Risico's van Nanodeeltjes" Rathenau Instituut.
- Peetoom, F, Peters, CJ, & Schoonman, J (2004). Hydrogen Storage in Gas Hydrates. gesprek met F. Peetoom, verschenen in H2World, Issue 2, Dec. 2004, pag. 10-12: Delft. interview / gesprek.
- Rolloos, B, & Schoonman, J (01-03-2004). Solar Energy - A Bright Future. TG Magazine, pp. 12-12.
- Schmidt-Ott, A & Ristovski, ZD. Measurement of Airborne particles. In Morawska, L, & Salthammer, T, (Ed.), *Indoor Environment*. (pp. 56-81), (2003) Weinheim: Wiley-VHC
- Schoonman, J (Ed.). (2004). *Nanotechnology Law & Business* 1 (1).
- Schoonman, J (2004, November ). Nanostructured materials for conversion and storage of sustainable energy. Rome, Italy, Plenary Lecture Present Situation and Forecasts of Nanotechnology in: Materials, Health and Medical Systems, Energy.
- Schoonman, J (2004, June ). Sustainable Energy and Hydrogen Economy. Brasov, Roemenie, Plenary Lecture First International Conference on ENvironmental EDUcation.
- Schoonman, J (2004, April ). Innovations in Energy Storage. Ambassadors Residence, Washington DC, Invited lecture Symposium "Sustainable Energy: the Dutch Perspective".
- Schrauwers, A, Ommen, JR van, & Nijenhuis, J. 'Chaotisch' manoeuvreren langs de afgrond. Delft Integraal, pp. 3-7.
- Schrauwers, A, Ommen, JR van, & Nijenhuis, J. Moving closer to the edge thanks to chaos. Delft Outlook, pp. 11-14.
- Wisman, R, & Schoonman, J (22-01-2004). De waterstofeconomie geeft gas. Memory Magazine, pp. 20-23.

### 3.2 Acquiring additional funding

Additional funding started in 2000

Funding source	Project title				man months				Total, not specified	Running budget	investment
		start	time	project	PhD	PD	UD	T	k€	k€	k€
NWO/CW open	Electroless Measurement of Photo-induced Charge Separation in Inorganic-Semiconductor /Conducting-Polymer Bilayers	01/01	4y	$F_e1$	48					5.5	68
NWO/FOM	Electroless Monitoring of Photoconductivity in Thin Conjugated Polymer Films	01/03	4y	$F_e1$	48					40	

Additional funding started in 2001

Funding source	Project title				man months				Total, not specified	Running budget	investment
		start	time	project	PhD	PD	UD	T	k€	k€	k€
EU-FP5	Self-Assembling and Self-Healing Electronic Devices Based on Discotic Materials; DISCEL LIBERAL	01/02	3y	$F_e1$		36			223		
		01/11	4y	$S_e1$		18		6	80		

Additional funding started in 2002

Funding source	Project title				man months				Total, not specified	Running budget	investment
		start	time	project	PhD	PD	UD	T	k€	k€	k€
NWO/CW jonge ch.	Theory of Charge Transport in Pi-stacked Systems including DNA	19/08	2.5y	$F_e1$		30					29
NWO-ACTS											
NWO/FOM	Excess Charges on Isolated Conducting Polymer Chains: Delocalisation and Motion	18/1	4y	$F_e1$	48						97
NWO-OTHER	Neutron beam time at ISIS (Oxfordshire)	01/01	2y	$F_e2$					210		
	Neutron beam time at ISIS (Oxfordshire)	01/01	2y	$F_e1$					225		
	Neutron beam time at ILL (Grenoble)	01/01	2y	$F_e2$					45		
	Neutron beam time at ILL (Grenoble)	01/01	2y	$F_e1$					60		
DPI	Nanocomposite hybrid solar cells	06/01	4y	$F_e1$	48					36	68

Additional funding started in the SENECU period – mentioned starting dates refer to 2004.

Funding source	Project title				man months				Total, not specified	Running budget	investment
		start	time	project	PhD	PD	UD	T	k€	k€	k€
NWO-ACTS											
NWO-VENI	Interstitial lithium-ion mobility in electrode compounds	01/09	3y	$F_e2$		36					
NWO-VICI	Ultrafast dynamics of excitons and charge carriers in functional materials	01/03	5y	$F_e1$	48	60					900
NWO-OTHER	Neutron beam time at ISIS (Oxfordshire)	01/04	2y	$P_e1$					225		
	Neutron beam time at ILL (Grenoble)	01/04	2y	$P_e2$					210		
NRSCC			4y	$S_e4/S_e5$	48				600		
SenterNovem-MKB	Ontwikkeling nieuwe technologie voor industriële productie van CuInS <sub>2</sub> dunnefilm zonnecellen op basis van (elektrostatische) sproeidepositie "(Full-sprayed zonnecellen)"	04/04	3y	$P_e1$					450		
SenterNovem-NEO	Early Agglomeration Recognition System II	07/04	1.5y	$P_H5$					100		
SenterNovem	Development of Turby windmill system – several projects			$P_e4$							
EET-Kiem	Development of the Electrostatic Wind Energy Converter I			$S_H6=F_e3$							
	Urban Turbines coordinated by Ecofys			$P_e4$							
EU-FP5	Self-Assembling and Self-Healing Electronic Devices Based on Discotic Materials; DISCEL	01/02/01	3y	$F_e1$		36			223		
	Biocellus			$P_H4=U_H2$							
	Crisgas			$P_H4=U_H2$							
EU-FP6	Alistore	01/01	5y	$S_e1$	48	36				90	150
	Two Very-High Thermal Reactor projects funded by the EC			$P_H6$							
	One Gas-cooled Fast Reactor Project (GCFR) funded by the EC			$P_H6$							
Industry	NRG, Petten: One Very-High Thermal Reactor project funded by Industry			$P_H6$							
	Sachtleben, D	08/04	6m	$P_H5$							
	Shell IEP	01/01	1y	$S_e1$					45		

**Knowledge valorisation and utilisation – dissemination of results**
**Brief overview of valorisation and utilisation**

<b>Dates</b>	<b>Type</b>	<b>Type of audience</b>	<b>Countries addressed</b>	<b>Size of audience</b>
17/09/04	Information address Costumer day Project info, equipment sharing	Toyota, Zaventum, B	All	6
16/06/04	Information address Costumer day Project info, equipment sharing	Shell Renewables, NL	All	10
24/09/04	Information address Costumer day Project info, equipment sharing	STW (technology foundation)	NL	10
23-24/ 11/04	Combined Workshop of SENEUCU and ALISTORE in Delft	R&D, S&T	All	100
11-12/04	Flyers – Superbus+ Project proposal address	Governmental on ministry level	NL	~5

#### 4. Personnel

The list of personnel is quite long and therefore, has been broken down in three parts, i.e. project leaders including the scientific director, permanent personnel, and temporary personnel.

##### Permanent personnel – project leader and scientific director (=program council)

	<i>Naam</i>	<i>Fte</i>	<i>Inzet</i>	<i>Faculteit</i>
HGL	J.Schoonman	1	0.5	TNW
	J. de Swaan Arons	0	0.05	Emeritaat
	T.H.J.J. van der Hagen	0.2	0.2	TNW
	G.J. Kearley	1	0.5	TNW
	I.M. de Schepper	1	0.1	TNW
	L.D.A. Siebbeles	1	0.1	TNW
	S. Picken	1	0.2	TNW
	J. Moulijn	1	0.15	TNW
	H. Spliethoff	1	0.3	ME
	J.A. Ferreira	1	0.5	EWI
	L. van der Sluis	1	0.1	EWI
	F. Hagen	1	0.1	TNW
	A. Schmidt-Ott	1	0.25	TNW
	UHD	H.J. Van der Kooi	0	0.1
F.M. Mulder		1	0.5	TNW
J.W. Metselaar		1	0.5	EEMCS
A.P.L.M. Goossens		1	0.2	TNW
J.C. Jansen		1	0.5	TNW
Van Bussel		1	0.2	LR
UD	E.M. Kelder	1	0.5	TNW
	J.R. van Ommen	1	0.25	TNW
	G. Mul	1	0.35	TNW
<b>Totaal</b>		<b>19.2</b>	<b>6.15</b>	

##### Permanent personnel

	<i>Naam</i>	<i>Fte</i>	<i>Inzet</i>	<i>Faculteit</i>
HGL	P.M. Sarro	1	0.5	EEMCS
	F. Kapteijn	1	0.1	TNW
UHD	J.L.Kloosterman	1	0.5	TNW
	S.W.H. De Haan	1	0.5	EWI
	M.J. Hoeijmakers	1	0.5	EWI
	G.C. Paap	1	--	EWI
	M. Zeman	1	0.5	EEMCS
	R.A.C.M.M. van Swaaij	1	0.5	EEMCS
	J.C.M. Marijnissen	1	0.25	TNW
	S. Luding	1	0.25	TNW
UD	D.Lathouwers	1	0.5	TNW
	P.C.M. Gubbens	1	0.2	TNW
	T.J. Savenije	1	0.5	TNW
	J.M. Schins	1	0.5	TNW
	F.C. Grozema	1	0.5	TNW
	N. Woudstra	1	0.5	ME
	P. Bauer	1	0.5	EWI
	H. Polinder	1	0.5	EWI
	P.J. Kooyman	1	0.1	TNW
	TO	A.M. van Voorden	1	0.5
J. Nijenhuis		1	0.2	TNW
<b>Totaal</b>		<b>21</b>	<b>8.1</b>	

## Temporary personnel

	<i>Naam</i>	<i>Fte</i>	<i>Inzet</i>	<i>Faculteit</i>	
Promovendus	S. Lems	1	0.9	TNW	
	B.Boer	1	0.9	TNW	
	W.F.G. van Rooijen	1	0.9	TNW	
	H.G. Schimmel	1	0.9	TNW	
	S. Fratiloiu	1	0.9	TNW	
	J.M. Huijser	1	0.9	TNW	
	P.A.C. Quist	1	0.9	TNW	
	P. Prins	1	0.9	TNW	
	K. van der Nat	1	0.9	ME	
	J. Morren	1	0.9	EWI	
	J. Popovic	1	0.9	EWI	
	M. Pavlovsky	1	0.9	EWI	
	M.B. Gerber	1	0.9	EWI	
	Dubois	1	0.9	EWI	
	G. van Elzakker	1	0.9	EEMCS	
	A.M.H.N. Petit	1	0.9	EEMCS	
	B.E. Pieters	1	0.9	EEMCS	
	A. Klaver	1	0.9	EEMCS	
	L. Simonin	1	0.9	TNW	
	M. Bartels	1	0.9	TNW	
	R. Loef	1	0.9	TNW	
	L. van Eijck	1	0.5	TNW	
	A.J.M. Schmets	1	0.6	TNW	
	O. Kruglova	1	0.9	TNW	
	Shibata	1	0.9	TNW	
	A. Galdhar	1	0.9	TNW	
	S.M. Mertens (tot 1-10-04)	1	0.9	CITG	
	C. Ferreira (vanaf 1-10-04)	1	0.9	LR	
	Post Doc	W. Knulst	1	0.9	TNW
		S.K. Kittusamy	1	0.9	TNW
R.J. Zambrano		1	0.9	EEMCS	
D.R. Simon		1	0.9	TNW	
U. Lafont		1	0.9	TNW	
M. Wagemaker		1	0.9	TNW	
Zhang		1	0.8	TNW	
P.P. Pescarmona		1	0.9	TNW	
Toegevoegd onderzoeker	P.V. Aravind	1	0.1	ME	
	H. Morita	1	0.1	ME	
	B. Roodenburg	1	0.9	EWI	
	F.G.B. Ooms	0	0.1	Extern	
<b>Totaal</b>		<b>39</b>	<b>32.8</b>		

## 5. Financial paragraph

A brief overview on the costs is given in the below table. The main deviations are mentioned as well. For convenience, the budget planning till 2006 has been given – a recall from the business plan.

### Financial overview for the years 2003 and 2004

	Spending k€	Budget k€	Major deviations from plan
<b>Personnel (fte)</b>			
Visiting Professor Research Fellow		(2)	
PhD Students	237 (7.5)	465 (11.4)	PhD students started later, and k€ 163 per 4 year was budgeted, will probably be k€ 155.
Post docs Projected permanent personnel	92 (2.1)	232 (4)	PD started later, and k€ 58 per year was budgeted, is probably k€ 50.
Added researcher Technicians		53 (0.8)	Not recruited yet, under discussion
<b>Subtotaal</b>	<b>419</b>	<b>750</b>	
<b>Investments and Materials</b>			
Components	23	46	See "Promovendi"
Travel & Subsistence	5	20	Only Scientific director travelled for SENEUCU.
Management <sup>(1)</sup>	60	98	Fixed amount, needs still to be transferred
Room of initiative	40	120	Will be consumed during the four years of funding
<b>Subtotaal</b>	<b>128</b>	<b>284</b>	
<b>Totaal</b>	<b>537</b>	<b>1034</b>	

<sup>(1)</sup> Management costs include also communication and reporting costs.

<sup>(2)</sup> Costs fall under "room of initiative", i.e. k€ 120.

Estimate according to business plan (recall)

Year	2003	2004	2005	2006	total
Personnel	28	722	618	572	<b>1940</b>
Consumables	1	45	41	39	<b>126</b>
Other	120	0	0	0	<b>120</b>
T&S	0	20	20	20	<b>60</b>
DISE	28	70	69	75	<b>242</b>
Total	<b>177</b>	<b>857</b>	<b>748</b>	<b>706</b>	<b>2488</b>

# **Delft Research Centre for Sustainable Energy**

*"SUSTAINABLE ENERGY, EXTRACTION,  
CONVERSION AND USE; SENEUCU"*

**ANNUAL REPORT  
August 2003- December 2004**

**ATTACHMENTS**

## ATTACHMENT I

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## ATTACHMENT II

Output continued.

**Refereed papers**

1. Au, S.F., S.J.McPhail, N. Woudstra, K. Hemmes, The influence of operating temperature on the efficiency of a combined heat and power fuel cell plant. *Journal of Power sources* 122 (2003), 37 – 46
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3. Burns, G., F. Favier, D. J. Jones, J. Roziere and G. J. Kearley. Potential Model for Tetrathiafulvalene Based on Inelastic Neutron Scattering and Raman Spectra. *J. Chem. Phys.*, 119, 4929 (2003).
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5. Debije, M.G., J. Piris, M.P. de Haas, J.M. Warman, Z. Tomovic, C.D. Simpson, M.D. Watson, K. Müllen, The optical and charge transport properties of discotic materials with large aromatic hydrocarbon cores, *Journal of the American Chemical Society*, 126 (2004) 4641-4645.
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8. Enache, C.S., Schoonman, J, & Krol, R van de. The Photoresponse of Iron- and Carbon-doped TiO<sub>2</sub> (Anatase) Photoelectrodes. *Journal of Electroceramics* 13, (2004)177-182.
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10. Erven, J.W.M. van & Marijnissen, J.C.M. The Production of Platinum Nanoparticles bij EDHA. *Journal of Aerosol Science* 34 (2003) S303-S304
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## ATTACHMENT III

**Verifiable targets Delft Research Centre for Sustainable Energy "SENECU"****1: Establishment of the Delft Institute for Sustainable Energy (DISE)***1.1 Targets and activities for the DRC and DISE.*

A clear description of targets and tasks will be prepared in a document for both the DRC and DISE. This description will include how DISE will carry out the projects as defined within the DRC SENEKU and how the relation will be established with other projects associated with DISE.

- The document will be delivered before the Mid-term assessment of the DRC.

*1.2 Contribution to shared education programs on sustainable energy.*

A shared education program associated with sustainable energy will play a significant role in order to attract students. Invited lectures on this subject will be given at Dutch and foreign universities. Within the 3TU-discussions, a new master course on this subject will be established.

- According to expectations the commencing date for this program is in the academic year 2006-2007.
- The "Energy master course" of the three TUs can take-off as soon as the decision is made within the 3 TU-discussion.

*1.3 Restructuring the use of (shared) research facilities.*

The research facilities of the participating research groups will be documented and this serves the creation of a plan for mutual use within the current and future research projects, thereby stimulating collaborations.

- The plan will be delivered at the end of 2005.

*1.4 Contribution to social acceptance of the use of sustainable energy resources, such as the introduction of a hydrogen economy.*

- Occasionally and frequently, a contribution will be given to publications and demonstrations concerning the social discussion associated with the acceptance of the use of sustainable energy resources – an example is the "SUSTAIN" symposium.

**2: Establishment of an integrated research program***2.1 Redefining of research directions and targets.*

Given the changing research directions of several departments participating in the DRC, the research directions and targets need to be adjusted or to be focussed.

- The modifications and adjustments will be finished mid 2005, depending on the pace of the local departmental changes.

*2.2 Programming of the use of shared equipment and facilities.*

Currently, no investment is foreseen in durable equipment for the DRC financed directly by TUDelft.

- After each calendar year, the financial situation will be reviewed in order to find out whether there is a possibility for additional investments.
- An annual overview will be made, listing all the equipment that is available for use, or eventually needs to be purchased for the research in this DRC, including also the purchase from external funds.

### 3: Acquiring of external funds and/or means

Acquiring external funds will be specified (for each cluster) in relation to existing subsidy programs. (Enrolled equipment will be mentioned as well.) Acquisitions will be done preferably multidisciplinary and within collaborations.

	TOTAL			
	man months			k€
	PhD	PD	OTH	
B-BASIC	48	12	0	0
NWO-ACTS	96	36	12	0
NWO-VENI	0	36	34	0
NWO-VIDI	0	0	0	0
NWO-VICI	96	60	0	900
NWO/FOM	96	0	0	0
NWO-ECHO	48	12	0	15
NWO-OTHER	96	0	0	0
SenterNovem-MKB	0	0	0	7.5
SenterNovem-NEO	0	72	0	120
EU-FP6	96	36	0	320
EU-Grants	0	0	0	0
Industry	96	24	0	60
<b>TOTAL</b>	<b>672</b>	<b>288</b>	<b>46</b>	<b>1422.5</b>

PD: PostDoc, OTH: Other personnel

General Total	
PhD (Positions)	14
PostDocs (Years)	24
Others (Years)	3.8
Additional Investments (k€)	1423
Number of EC-projects	6

### 4: Dissemination Activities

#### 4.1 *Electronic publication*

Publications via internet are associated with the way the DRC will operate and is structured, and thus includes the projects to be carried out.

- The web site of SENEUCU will be ready mid 2005.

#### 4.2 *Scientific publications*

Within SENEUCU, it is the aim to have an annual increase of peer-reviewed shared publications by 20%.

- For 2005, the number of peer-reviewed shared publications will be five.
- For 2005, the number of PhD theses will be four and for 2006 it is projected to be five. The total number of publications will be 25. For 2006 these numbers will be 15 and 40, respectively.
- Mid 2006, an MRS book series will be published on Nanotechnology associated with energy research, Eds. E.M. Kelder and E. Leite
- The publication of books will be stimulated.

#### 4.3 *Presentations of the research at workshops, conferences, symposia etc.*

- DISE will organize a (shared) workshop every year – sharing with for instance the NoE "ALISTORE", or with other DRCs.
- For 2005, the number of invited lectures will be 25, and for 2006 40. Conference contributions will be beyond these numbers

### 5: Utilization

Based on the results of the research, several patents may be filed, also certain parts of the research may be of interest for implementation in industry.

#### 5.1 *Utilization of the results*

- The workshops will be used to invite the industry in order to create a platform for valorization.
- Industry oriented customer days will be organized on a regular basis or whenever applicable.

#### 5.2 *Patents*

- Patents based on catalysts for hydrogen storage
- Patents based on the use of Ionic Liquids in Li-ion batteries
- Patents based on 3D solar cells.

### 6: Management activities

The management activities are described in the business plan (Provisions) and the actual work done will be briefly addressed in the annual report.

#### 6.1 *Program and project review and assessment*

- An annual self-assessment will take place, based on these verifiable targets.
- A plan will be prepared for the up-coming year.
- A long-term scenario will be included into the future projections.

#### 6.2 *Reporting*

- An annual report will be prepared according to the TUDelft DRC template.

#### 6.3 *Financial part*

The financial administration of DCT/TNW co-ordinates the financial part of both DISE and the DRC.

- The financial administration will prepare an overview of the expenditures every quarter.
- For the annual report, a financial overview will be prepared, that may be used to propose possible investments.