DIFFER

STRATEGIC PLAN
2017-2022

WE ARE DIFFER. **SCIENCE FOR FUTURE ENERGY**

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PREFACE

It is with great pleasure that I present the Strategic Plan of the Dutch Institute for Fundamental Energy Research, one of the nine research institutes of the Netherlands Organisation for Scientific Research. This plan was prepared as part of DIFFER's external evaluation in 2017 and will guide the institute on its new mission from 2017 to 2022.

Public support to forge ahead with the energy transition is at an all-time high, matched by the growing awareness that existing technology alone will not be enough to create a fully sustainable energy system. Crucial, fundamental challenges need to be overcome in order to realize a flexible, sustainable energy infrastructure by the end of the century. DIFFER is fully committed to meeting this grand societal challenge. Our new and expanded mission directs us to perform leading fundamental research on materials, processes and systems for a global sustainable energy infrastructure, in close partnership with (inter)national academia and industry.

The newly hired researchers in our Solar Fuels research theme explore novel approaches to convert sustainable energy into CO_2-neutral fuels and chemical products. This research theme was set up in the previous strategic period and has already generated impressive first results. With access to their newly delivered, state of the art laboratories, this multidisciplinary theme will certainly make a major contribution towards realizing seasonal energy storage, long distance mobility and electrification of the chemical industry.

Prospects are equally good for DIFFER's established research theme on Fusion Energy. With our in-house linear plasma generator Magnum-PSI, we stand ready to validate materials choices that can withstand the extreme conditions expected in the nuclear fusion project ITER. Together with a strong effort on modeling, diagnostics and control, we will develop advanced concepts and scenarios for the even more intense conditions in DEMO fusion power plants beyond ITER.

In addition to providing valuable insights in Solar Fuels and Fusion Energy, we will also apply our cross-cutting, multidisciplinary approach in an exploratory program on other technologies for sustainable energy storage and power generation. The newly set-up Ion Beam Facility and Center for Computational Energy Research bring together the expertise to study materials and processes in active energy devices on a variety of length and time scales. This will generate insights valuable for a wide array of energy solutions.

DIFFER's leading position in Dutch energy research is matched by our strong ties to (inter)national research collaborations and agendas. As NWO's premier strategic instrument on energy research, DIFFER will continue to connect the various disciplines and actors in energy research and build a cohesive community for fundamental energy research.

I am convinced that the strategy put forward in this document will place DIFFER in an excellent position to make a real difference in energy research. Our well established focus on Fusion Energy and Solar Fuels and our new research facilities for broader explorative energy research will result in major contributions to fulfilling future energy needs. With a national leading and coordinating role, DIFFER will bring the Netherlands to the forefront in the international energy research arena.

I would like to thank all those who contributed to this document as well as all those who put their confidence in our institute fulfilling its challenging new mission.

Richard van de Sanden, Director
Eindhoven, June 2017

1 MISSION AND STRATEGIC OUTLOOK

The *Dutch Institute for Fundamental Energy Research* (DIFFER) plays a key role in the Dutch research landscape as the foremost strategic instrument in fundamental energy research of the Netherlands Organisation for Scientific Research NWO, the Dutch national science agency. DIFFER, one of nine dedicated NWO research institutes, was established in 2011 as the successor to the FOM Institute for Plasma Physics 'Rijnhuizen'.

1.1 Mission

DIFFER's ambition is to support society in meeting the challenges of global warming and rising energy demand. Both require an energy infrastructure that is able to fulfill energy requirements in a CO_2-neutral manner by the year 2050. Fundamental, cross-disciplinary scientific research is crucial for the development of new sustainable technologies that can meet these grand challenges and transform our current, fossil fuel dominated energy infrastructure.

DIFFER's mission therefore is

> *To perform leading fundamental research on materials, processes and systems for a global sustainable energy infrastructure, in close partnership with (inter)national academia and industry.*

In short, DIFFER performs "*Science for Future Energy*".

1.2 DIFFER's guiding principles

DIFFER is in an excellent position to fulfil its mission. It demonstrates a strong performance in all four key aspects that can be considered the guiding principles for operating a successful research institute (and which are recognized as such by NWO, the Dutch national science agency - see sidebar DIFFER and the national research strategy):

I Scientific excellence

DIFFER is an internationally acknowledged center of expertise in fundamental energy research and performs at the world's top level in its field. The institute boasts excellent research groups with multi-disciplinary expertise in physics, chemistry, materials science and computational science, staffed by talented researchers. DIFFER executes scientific programs at a scale and speed that cannot be realized at the individual Dutch universities. Adding to this, DIFFER maintains an agile governance enabling the institute to rapidly form research teams when a scientific challenge needs urgent attention, or dissolving teams when insufficient resources slow down a project or when (scientific) progress is slow.

II World-class research infrastructure

DIFFER develops and exploits a comprehensive in-house research infrastructure and facilitates its use by third parties. It comprises the world class Plasma Surface Interactions or PSI facilities (including the crown jewel Magnum-PSI), Ion Beam facilities (IBF) and a wide variety of state-of-the art labs. Dedicated and highly qualified technical staff ensure that the facilities operate at top-level. In addition to its in-house experiments, DIFFER also participates in internationally leading nuclear fusion research laboratories and is the gateway for domestic academic groups to these large-scale international facilities.

Sidebar 1: Societal relevance

Research at DIFFER serves society in its efforts to develop CO$_2$-neutral energy systems, thus mitigating the influence of human activity on global warming as was established by the Intergovernmental Panel on Climate Change (IPCC). The global ambition agreed upon in the Paris Agreement[1] is to limit global warming to less than 2 degrees Celsius (°C) compared to pre-industrial levels. This calls for zero net CO$_2$ emissions to be reached during the second half of the 21st century and thus requires a transition towards a fully sustainable energy supply. By performing fundamental, cross-disciplinary research in the fields of Solar Fuels and Fusion Energy, DIFFER can make significant contributions to the crucial phases of the energy transition in the coming decades.

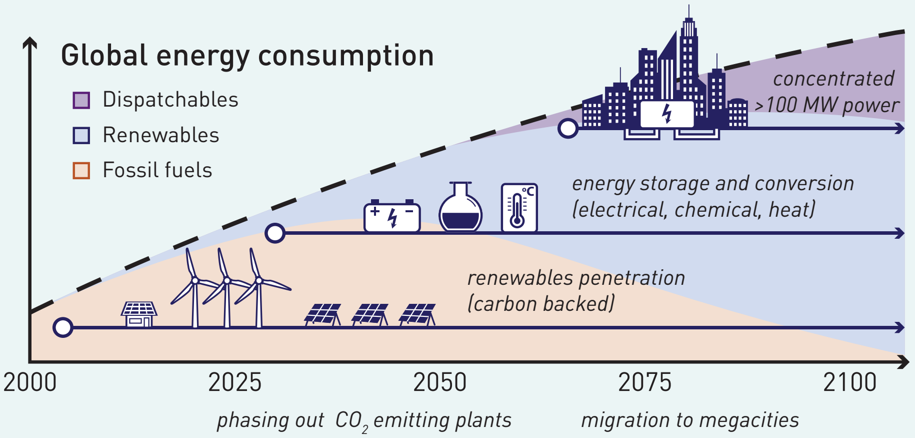

Figure 1.1. The energy transition and its demands on technology and research.

The current phase of the energy transition is characterized by the rapid penetration of solar and wind into the energy generation mix. The inherent intermittency of these technologies is being overcome mainly by the deployment of existing fossil fuel-based combustion technology. In the next phase this back-up power can be provided in a CO$_2$-neutral manner by new combustion plants with technology for carbon capture and storage (CCS), and by new technologies for storage of electricity: ***solar fuels*** *and batteries. In the third phase the energy system will have to meet the needs of increasing numbers of megacities (over 10 million inhabitants) that are expected to emerge towards the end of the century. These requires safe, localized, dispatchable sources of CO$_2$-neutral energy, which can be provided by inherently safe nuclear technology such as* ***nuclear fusion*** *and generation IV nuclear fission (e.g. thorium molten salt reactors).*

DIFFER also establishes societal relevance by its modus operandi where strong contact with high-tech SME's and industry is essential, both as an inspiration for research questions and to translate results of fundamental research into practical applications. Furthermore, DIFFER strongly advocates the importance of fundamental energy research in relevant industrial and governmental networks and reaches out to politics, media, schools and the public at large.

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[1] Paris Agreement (UNFCC 2015) http://unfccc.int/paris_agreement/items/9485.php

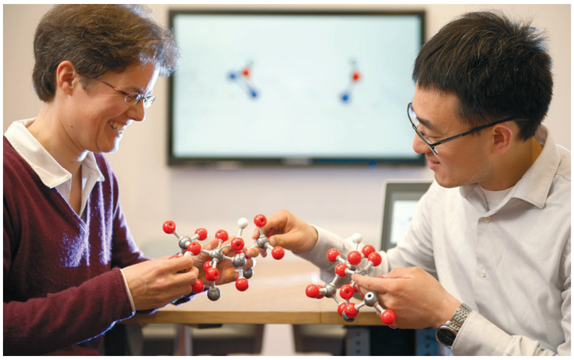
III Facilitating and coordinating role

DIFFER promotes cohesion in fundamental energy research in the Netherlands. The institute initiates, executes and leads research networks across scientific disciplines and technological readiness levels. As a partner in the Netherlands Energy Research Alliance (NERA), DIFFER contributes in international agenda-setting fora such as the joint programs of the European Energy Research Alliance (EERA) and ensures an optimal connection of Dutch science to international energy research. DIFFER is the national home base for nuclear fusion research through its membership of the Horizon2020 program EUROfusion.

IV Connecting science and industry

To turn fundamental insights into innovative solutions for the energy challenge, it is imperative for scientific, economic and societal partners to collaborate. DIFFER plays an active role here by connecting science and higher education, small and medium enterprises and high-tech industry through public-private partnerships and through the formation of (strategic) research programs and networks.

I. Scientific excellence



II. World-class research infrastructure

III. Facilitating and coordinating role

IV. Connecting science and industry

1.3 Strategic goals

Based on its mission and following up on the aspects listed above, DIFFER has formulated the following strategic goals for 2017-2022:

- To focus on **fundamental research,** enabling solutions for energy generation, conversion, storage and transport for future sustainable energy systems, in **a programmatic and integral approach**, exploiting the various research disciplines and high tech infrastructure available in the institute.

- To **maintain and further develop its research infrastructure** in order to facilitate research at the forefront of science.

- To serve as a focal point for (inter)national energy research and to **connect networks of scientific, educational, industrial and societal partners.** Whenever possible, DIFFER will seize or create opportunities for use-inspired research programs on energy-related topics with enterprises and industry, for knowledge transfer and valorization. DIFFER aims at a facilitating and/or organizing role regarding the coordination of energy research in the Netherlands.

- To maintain a **viable, healthy organization** with a diverse, highly educated, well trained staff, a sound financial strategy, and a healthy working environment.

Through the further development of its research programs in close collaboration with its partners, the deployment of experimental facilities with unique capabilities, its highly qualified staff, and its extensive network, DIFFER will continue to bring the Netherlands to the forefront in the international energy research arena.

Sidebar 2: DIFFER and the Dutch national research strategy

DIFFER's focus on fundamental energy research embodies the important role that NWO has identified for physics, chemistry, materials science and computational science to play in the energy research theme[2]*. DIFFER follows NWO's guidelines for institutes*[3]*, i.e. providing focus and mass to the related field through excellent research, housing of international research facilities,maintaining strong collaborations with universities, the business community and society, and acting as focal point in their areas of expertise and as regional knowledge partners.*

A good example of acting as focal point is DIFFER's initiative (under the umbrella of the Netherlands Energy Research Alliance, NERA) of The Energy Transition route[4] *within the Dutch Science Agenda*[5]*, which describes ten challenges to be covered in long term research programs*[6]*.*

DIFFER's relevance for the national research strategy is furthermore illustrated by its active collaboration with societal partners.It participates in all three so-called Topsectors (the Dutch government's instrument to promote collaborations between industry, SME's and academiain the fields of Energy, Chemistry and High Tech Systems and Materials[7]*, respectively), its key partnership in NWO's Industrial Private Partnership programs (together with Fujifilm Research, Philips Lighting and Syngaschem BV) and in an M2i public private partnership with ASML, NRG/ECN, and Research Instruments.*

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[2] Vision document Chemistry & Physics in 2025: http://www.nwo.nl/actueel/nieuws/2013/cw/visiedocument-chemie-en-natuurkunde-in-2025-aangeboden.html
[3] NWO Strategy 2015-2018: http://www.nwo.nl/over-nwo/X+publicatie/nwo/strategienota-2015-2018.html and the FOM strategy 2015-2019.
[4] The NWA route "Energy Transition" http://www.wetenschapsagenda.nl/energietransitie/
[5] The Dutch National Research Agenda (NWA) developed an overview of societally relevant research in the Netherlands. Societal partners and members of the general public entered 12,000 questions to science, which were collected in 25 cross-disciplinary Routes (research agendas).
[6] Adding to this, DIFFER director Prof. M.C.M. van de Sanden was appointed chairman of the NERA Science Board
[7] The Topsector policy: https://www.topsectoren.nl/publicaties/brochures/2016/03/16/hoe-en-waarom-topsector-engels. The DIFFER research has most relevance for the roadmaps of the Topsector Energy, Topsector Chemistry and Topsector High-Tech Materials & Systems (HTSM).

SWOT analysis DIFFER

In preparation for this Strategic Plan, DIFFER performed a SWOT analysis, identifying internal and external factors that can aid or hinder in achieving its goals. This analysis is presented below.

Strengths

- High quality and focus of research program with an integrated approach and overarching use of techniques and methods in both Solar Fuels and Fusion Energy research.
- Strong position in computational science.
- Well connected to the European nuclear fusion research community; access to world class (inter)national facilities.
- Highly professional, international scientific staff with multidisciplinary background and track record in energy research.
- World class PSI lab; high quality infrastructure operated by highly professional technical staff; excellent workshop and support facilities.
- Flexible research facilities in the new building enable swift exploration of new research directions.
- Good funding base where strategic program funding is secured within the mission budget combined with a strong position in acquiring public-private funding.

Weaknessess

- Substantial fraction of scientific staff has been appointed recently and is not yet very visible in the scientific community.
- Lack of gender diversity; low ratio of female staff in leadership positions.
- Technical staff is dominantly trained in physics whereas also other disciplines are required (materials engineering, chemical, nuclear analysis, advanced laser techniques).
- The number of personal grants (NWO-VI, ERC grants) although increased in 2011-2016, is still relatively low.

Opportunities

- Societal need for conversion and storage of renewable electricity; sustainable energy research is high on (inter)national agenda.
- Increased funding for the energy transition and the electrification of the (chemical) industries.
- Ion beam facility uniquely positioned to study in situ and operando interfaces (under extreme conditions) in energy systems.
- New Center for Computational Energy Research will open new research lines and collaborations.
- Worldwide unique facilities and technologies both at DIFFER and other Dutch knowledge institutes, such as the Reactor Institute in Delft and the Space research institute SRON, justify a national nuclear fusion research program.
- Facilities on plasma-surface interaction coming online elsewhere offer specialization and collaboration opportunities.

Threats

- 'Climate skepticism' could lead to less attention for (fundamental) energy research to mitigate atmospheric CO_2 levels.
- If ITER and EUROfusion programs would be stopped, research into energy from nuclear fusion becomes challenging to continue.
- Difficulty to keep and recruit top-level PhD engineers and skilled technical personnel because of competing opportunities in the Eindhoven region.
- Lack of coordination in fundamental energy research in the Netherlands, leading to scattered research initiatives.
- The new NWO organization makes strategic program funding more difficult to organize.

2 STRATEGIC CHOICES AND ACTIONS

Building on DIFFER's excellence in research, its world class infrastructure and its strong position in the (inter)national energy research community, the prospects of achieving the strategic goals described in the previous chapter can be considered as good. Nevertheless, to succeed in fulfilling its mission, it is paramount for DIFFER to make the right strategic choices and take appropriate actions.

2.1 Research choices

Three major societal developments affect the DIFFER research strategy:

- ***The acceleration of the transition towards a CO_2-neutral energy society*** according to the targets set for 2030 and 2050 by the international Paris COP 21 agreement (UNFCCC)[8], by the EU (RED)[9] and nationally (Energieagenda)[10]. Therefore the reduction of CO_2 emissions will be the overriding driver to provide innovative energy solutions.
- ***The urgent need for storage of renewable electricity***. In the coming years surpluses are expected in several European countries (see box), resulting in an imbalance in the power grid. A power grid imbalance can only be overcome by diverting renewable electricity into other parts of the energy system powered by oil, gas, coal or chemicals.
- ***The need for centralized, dispatchable[11], CO_2-neutral power generation***. The transition towards CO_2-neutral energy supply will proceed in parallel with demographic changes leading to the majority of the world's population living in urban areas. A robust sustainable energy infrastructure able to accommodate the needs of future mega-cities will require technology for dispatchable, CO_2-neutral central power generation.

Fundamental research is crucial for society to meet these challenges, enabling innovative and viable energy solutions. DIFFER contributes to this with its multi-disciplinary expertise in physics, chemistry, materials science and computational science. Focusing on the two research themes Solar Fuels and Fusion Energy, each in itself providing solutions for the energy challenge, DIFFER maintains an integral approach where cross-fertilization and collaboration are in the institute's DNA. As a result DIFFER is able to broaden the research portfolio through explorative projects and programs that contribute to the much needed acceleration in the development of energy solutions within and beyond the two themes that are at the heart of the DIFFER research.

a. Solar Fuels

The DIFFER Solar Fuels research has the potential to contribute to the much needed acceleration in the development of enabling technologies for the transition towards a CO_2-neutral energy society. In this respect the outlook on an integrated solar fuels device that directly converts sunlight into chemicals and fuels, with minimal losses in the subsequent steps, remains appealing. This concept is subject of intensive research globally[12] and will continue to be investigated within the DIFFER research program. However, this research has progressed at a much slower pace than originally anticipated and will most likely not have a large impact on the energy

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[8] Marrakech Action Proclamation for Climate and Sustainable Development (UNFCCC, 2016), https://unfccc.int/files/meetings/marrakech_nov_2016/application/pdf/marrakech_action_proclamation.pdf

[9] Directive 2009/28/EC of the European Parliament and the Council (European Union, 2009), https://ec.europa.eu/energy/en/consultations/preparation-new-renewable-energy-directive-period-after-2020

[10] Energieagenda (Dutch Ministry of Economic Affairs, 2017), https://www.rijksoverheid.nl/documenten/rapporten/2016/12/07/ea

[11] https://en.wikipedia.org/wiki/Dispatchable_generation

[12] Joint Center for Artificial Photosynthesis (JCAP), http://solarfuelshub.org, Solar Fuels Institute (SOFI), http://www.solar-fuels.org; Advanced Materials and Processes for Energy Application (AMPEA), https://www.eera-set.eu/eera-joint-programmes-jps/advanced-materials-and-processes-for-energy-application-ampea/

transition before 2030. It has become clear that to directly convert photons and chemical building blocks into fuels and chemicals, breakthroughs and novel concepts are needed that (amongst others) enhance photon absorption and charge carrier generation; prevent charge carrier recombination; and improve charge transport. In DIFFER's Solar Fuels research program the focus on these challenges using disruptive nano-photonic and plasmonic approaches will be further pursued.

The growing need to divert surplus renewable electricity to parts of the energy system that are currently powered by fossil fuels and chemicals has spawned a renaissance in the development of innovative electrochemical processes[13]. The JCAP consortium in the US, originally focusing on artificial photosynthesis and photo-electrochemical devices, but also large consortia and programs in USA, Germany, France and Denmark, are now investigating scalable electrochemical processes that can convert electricity directly in dense energy fuels and chemicals using the chemical building blocks CO_2, N_2 and H_2O[14]. Since these electrochemical conversion processes are usually hampered by the selectivity and activity of the electro-catalytical processes used[15], this provides DIFFER with a great opportunity to broaden its Solar Fuels research program towards these aspects (and not necessarily focus only on fuels for energy storage). DIFFER's expertise and research facilities put the institute in an excellent position to strengthen this research field and provide solutions, in particular through a focus on the integration of non-thermal (plasma-)chemical processes with nano- and micro-structured functional materials; and interfaces in (photo-)electrochemical devices.

In summary, DIFFER's Solar Fuels research is in an excellent position to provide key contributions to renewable electricity driven chemistry for the production of chemicals and fuels starting from CO_2, H_2O and N_2. There are also ample opportunities to apply the DIFFER Solar Fuels expertise in other fields of sustainable energy conversion and storage.

Solar Fuels

Storing solar energy in chemical form

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[13] Elektrifizierung Chemischer Prozesse, https://dechema.de/dechema_media/Dechema_DiskPap_Elektrifizierung_2015-p-5905.pdf; Electrification in the Dutch process industry, http://topsectorenergie.nl/wp-content/uploads/2017/03/Electrification-in-the-Dutch-process-industry.pdf

[14] Carbon2Chem program (Germany), https://www.thyssenkrupp.com/de/carbon2chem, ARPA-E programElectrofuel (USA), https://arpa-e.energy.gov/?q=arpa-e-programs/electrofuels; Kopernikus program (Germany) https://www.kopernikus-projekte.de/projekte/power-to-x

[15] An example is the replacement of the NH_3 production process Haber-Bosch process by an electrocatalytic process using H_2O and N_2. The selectivity for ammonia production is less than 1%. Aayush R. Singh et al., ACS Catal. **7,** 706 (2017)

Sidebar 3: The concept of Solar Fuels

Solar fuels are energy carriers (such as methane, alcohols, ammonia and synthetic hydrocarbons) synthesized with solar energy from sustainable raw materials such as water (H_2O), carbon dioxide (CO_2, obtained from sustainable sources, ideally from air capture), and/or nitrogen (N_2), as is illustrated in the figure below[#]. These chemicals and fuels are CO_2-neutral and have a large potential for sustainable energy storage. As an alternative to dense energy carriers, also industrially relevant chemicals can be synthesized (like acids, aldehydes, and others).

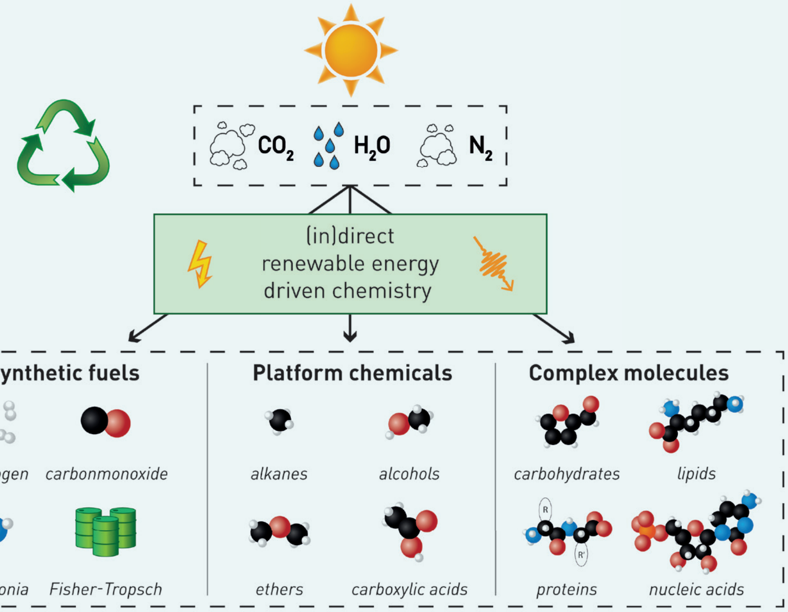

Figure 2.1. (In)direct conversion of sustainable energy and building blocks into synthetic fuels, platform molecules and complex molecules.

Direct routes for solar fuel production use solar light or heat as input (e.g. biofuels, concentrated solar power (CSP), artificial photosynthesis, photo-electrochemical cells), indirect routes have renewable electricity as input (e.g. from wind, solar or hydro power). Both direct and indirect routes have their applications. For example indirect routes align well with the dependence of modern societies on electrification, providing storage for surplus electrical power. Direct routes hold a potential for (cheaper) production of fuels using solar energy in remote locations.

Solar fuels produced from CO_2 effectively recycle CO_2 so their synthesis is often referred to as carbon capture and utilization (CCU).

[#] Alternatively, biomass can be used as a "chemical building block" for this scheme.

b. Fusion Energy

The discrepancy between the time scale for the transition towards a CO_2-neutral energy system (2050) and that of nuclear fusion technology contributing to the energy supply (2070-2100) introduces a new perspective on the development path of nuclear fusion energy. It must be motivated by the demands and requirements of the energy system at the time of its introduction.

The future energy system will be dominated by electricity generation from wind and PV, which is ruled by nature rather than demand. Intermittent wind and solar electricity already cause strain on the electricity grid as a result of the mismatch between supply and demand. This calls for a systems approach in which the focus is not just on the generation of sustainable energy, but where energy storage and energy transport form an integral part of the system. However, even when measures are taken to balance the natural seasonal and regional discrepancy between electricity supply and demand (such as a significant energy storage and conversion capacity, over-dimensionalizing of the renewable electricity generation system and smart grids), it remains questionable whether renewable energy production can match the required base load.

A recent analysis and extrapolation of the current German energy production system suggests that due to intermittency only ~40% of the base loadcan be provided for[16]. According to this analysis additional CO_2-free electricity production units will have to be available. In a global perspective this need will become even more important given the demographic trend towards urban settlements and increasing prosperity. Towards the end of the century a strong growth is foreseen in the number of megacities with immense energy needs. A cost-competitive fusion energy system can provide for CO_2-neutral dispatchable power generation, and, because of its high-energy-density, minimizes the impact on land use. This motivates the continued effort for the development of nuclear fusion technology, which has the added advantage of being inherently dispatchable. Additional fusion reactors can also cater to the need for high temperature heat and chemicals of the industry surrounding future megacities. Interestingly, the solar fuels, introduced in the generation mix to abate the intermittency of the renewables can now be used to improve the business model of nuclear fusion plants.

To accelerate the development of nuclear fusion energy, several "Smaller, smarter and faster" concepts have been proposed[17]. These include tokamak designs exploiting recent advanced superconducting magnet technology development[18], as well as non-toroidal concepts partly funded through the ARPA-E program[19]. Since these concepts require higher particle and heat confinement than ITER and DEMO, the plasma exhaust challenge is more intense, and new solutions are needed to dissipate the heat flow before it reaches the divertor. This implies that research into divertor materials and plasma solutions for plasma exhaust control (see sidebar), is also paramount for establishing the feasibility of new concepts in nuclear fusion energy. Adding to this, establishing an optimized plasma regime of operation is vital regardless of device size. DIFFER and collaborators can make meaningful contributions to both challenges, as they have proven excellence and expertise in plasma diagnostics, modeling, material research and control engineering.

Other advanced, inherently stable, low waste energy production systems include next generation fission reactors (e.g. generation IV). DIFFER is excellently positioned to take up the research challenges accompanying the development of such future energy production systems. Next generation reactors will require new generations of extreme materials that can function under the extremes of high temperature, high neutron flux and aggressive chemical corrosion[20, 21].

Fusion Energy

Clean and safe dispatchable energy

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[16] F. Wagner, Eur. Phys. J. **129**, 20 (2014), F. Wagner, Eur. Phys. J. Plus **131,** 445 (2016)

[17] http://sciencenetlinks.com/videos/smaller-faster-cheaper-route-fusion-energy/

[18] For example the MIT ARC proposal, B.N. Sorbomet al., Fusion Engineering and Design 100 (2015) 378–405

[19] https://arpa-e.energy.gov/?q=arpa-e-programs/alpha

[20] Technology Roadmap Update for Generation IV Nuclear Energy Systems, GEN IV International Forum, https://www.gen-4.org/gif/jcms/c_9260/public

[21] Basic Research Needs for Materials under Extreme Environments, report of the Basic Energy Sciences Workshop for Materials under Extreme Environments, Office of Basic Sciences, DOE, February (2008), https://science.energy.gov/~/media/bes/pdf/reports/files/muee_rpt_print.pdf

In summary: DIFFER's Fusion Energy research will provide key contributions to the challenges of the power exhaust and plasma regimes of operation of nuclear fusion reactors, and diversify its research on materials under extreme conditions towards other, non-nuclear fusion (energy) systems.

Sidebar 4: The plasma exhaust in magnetic confinement nuclear fusion

Next generation fusion reactors (such as ITER and its successor DEMO) will rely on a magnetically confined toroidal plasma with a core temperature of ~200 million K and a core electron density of 10^{20} m^{-3}. An essential element in these reactors is the exhaust for the continuous removal of impurities including the helium fusion reaction product. It is realized by diverting magnetic field lines from the edge of the reactor (the scrape off layer, SOL) to a remote surface in the divertor region, where the diverted plasma is neutralized and pumped away (see the figure below illustrating the situation for ITER).

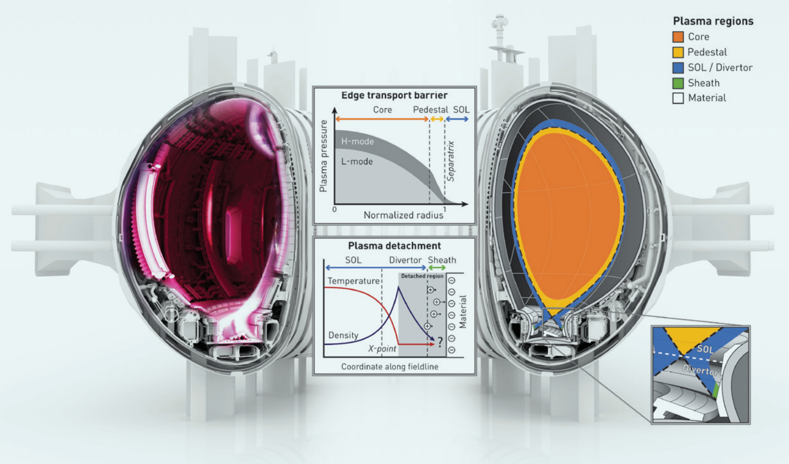


Figure 2.2. The plasma exhaust in magnetic confinement nuclear fusion.

A major concern in this approach is the concentration of the exhausted heat onto a small area of the plasma-facing material. In fact, the solution for the plasma exhaust is considered one of the most prominent challenges for controlled nuclear fusion. The routes outlined to provide a solution can be roughly categorized as:

- *controlled decrease of the plasma heat and particles load to the wall;*
- *by applying advanced magnetic configurations, avoiding or ameliorating instabilities in the plasma periphery (the so-called Edge Localized Modes), and through enhanced radiation by impurity injection;*
- *load-resilient reactor materials;*
- *validating materials and cooling concepts for the construction of the divertor in ITER and designing innovative materials solutions, such as liquid metals, for DEMO.*

c. Opportunities for new program development

Through the pooling of DIFFER expertise and experimental facilities, a unique and successful cross-cutting approach has emerged (see sidebar Cross-cutting approach) which puts the institute in a position to contribute to sustainable energy research in a broader perspective, beyond the themes described above. It enables DIFFER to diversify its research portfolio by means of explorative programs and projects.

DIFFER is especially well positioned to study materials and interfaces under extreme conditions, which is paramount for future energy technologies. Both enhancing the efficiency of existing technologies and developing new energy technologies will require materials resistant to extremes e.g. in temperature, chemical reactivity, photon or radiation flux, and electric or magnetic fields. The power exhaust in a tokamak nuclear fusion reactor is a striking example of an extreme environment, as are electrochemical systems (batteries as well as photo- and plasma assisted electrochemical systems) where materials, interfaces and catalysts will experience extreme conditions (high temperature and current densities) when scaled-up to higher power levels. Already in 2014 DIFFER initiated a program together with the Eindhoven University of Technology on the processing of materials under extreme conditions and in 2016 this was further explored in the granted program together with M2i. Next-generation nuclear fission reactors are another example of extremely demanding future energy technologies. For example the concept of IVth generation molten salt fission reactors and the liquid metal divertor concepts in nuclear fusion reactors share similar challenges in that respect.

In general the targeted design of new materials and processes requires an approach of analysis, synthesis/design and control. Through systematic performance studies the crucial synthesis/design parameters are identified after which an active control strategy can accurately establish these parameters during the process. Computer modeling and simulation supports this approach both in understanding the materials and process performance and in developing methods for control. On the horizon of such studies are new classes of materials and processes with greatly enhanced performance for future energy technologies: extending lifetimes, increasing efficiencies, providing novel capabilities, and lowering costs. DIFFER is, for instance, already preparing to engage (on a small scale, and in collaboration with SME's) in explorative projects on flow batteries (in particular low temperature NaS battery).

In summary: DIFFER's expertise and facilities are excellently aligned to further develop its cross-cutting research approach featuring in situ *and* operando *studies, multi-scale modeling and development of methods for active control. This will strengthen DIFFER's position to diversify its research portfolio and make a real difference in use-inspired fundamental research for sustainable energy systems.*

Sidebar 5: Cross-cutting approach

The following three distinctive elements are common to all DIFFER's research activities (as illustrated in the highlights in chapter 3) and constitute its cross-cutting research approach:

- **In situ *and* operando *studies*** *to reveal interface and/or material properties during operation and in relation to system performance. Transient phenomena that disappear in absence of the interacting environment are often most important for the understanding of underlying mechanisms and dynamics.*
- ***Multi-scale modeling*** *is important as a variety of physical phenomena is at play over wide ranges of length and time scales.*
- *Active control is a crucial aspect when it comes to applying the insights obtained through experiments and modeling to the development of real energy conversion systems and devices.*

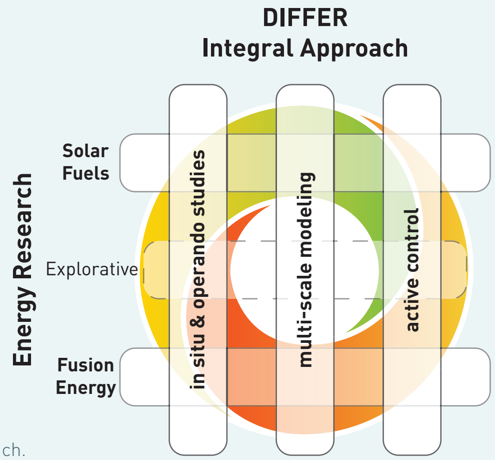


Figure 2.3. DIFFER's cross-cutting research approach.

2.2 Other strategic choices

Since performing research is the raison d'être of the institute, the future of DIFFER for the larger part depends on the strategic choices described above. However, focusing on research alone does not yield a viable institute. Therefore the strategic goals described in the previous chapter also pinpoint the other essential aspects of establishing a successful institute.

Regarding the crucial effort of maintaining and developing the state-of-the-art infrastructure, which is by all means closely connected to the choices in research, DIFFER will continue to exploit its strengths in designing, developing and operating mid-sized experimental equipment with a focus on *in situ* and *operando* studies of materials under extreme conditions. Equally important are facilities for multi-scale modeling and the development of methods for active control.

To further secure and strengthen its position as a leading research institute in fundamental energy research DIFFER will maintain close collaborations with its partners in academia, industry and society and play an active organizing and facilitating role in the energy research community.

Complementing all the efforts above and contributing to the successful continuation of DIFFER as a viable institute is the strategy to establish a healthy organization with a diverse, highly qualified workforce and a sound financial strategy.

2.3 Strategic actions

Based on the DIFFER mission and strategic goals, following up on the SWOT analysis and building on the choices described above, DIFFER has identified the following strategic actions for the period 2017-2022. They are listed according to the key elements of the strategic goals and will be further elucidated in the following chapters of this Strategic Plan.

Strengthening and further developing research in a programmatic and integral approach

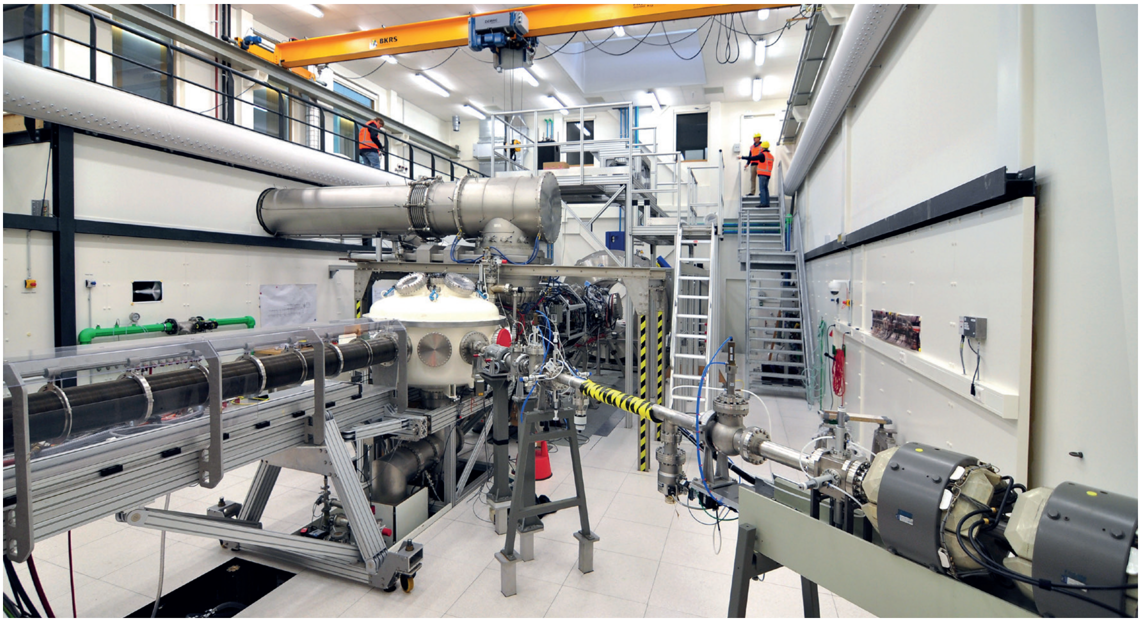
(see chapter 3)

- DIFFER will further intensify the focus of its Fusion Energy research on plasma physics, plasma chemistry and material solutions for the exhaust of nuclear fusion reactors.
- DIFFER will further intensify its focus on sustainable energy driven chemistry, using sustainable energy (photons and electrons) for the synthesis of fuels and chemicals.
- DIFFER will direct resources to explore fundamental research challenges outside the research focus of Fusion Energy and Solar Fuels, in order to diversify the research portfolio and be able to incorporate novel developments in energy generation, storage and conversion.
- DIFFER will further develop its cross-cutting research approach featuring *in situ* and *operando* studies, multi-scale modeling and development of methods for active control to meet the urgent challenges in sustainable energy systems.
- DIFFER will establish a new research group on control engineering and systems identification for energy systems.

Maintaining and further developing the research infrastructure to stay at the forefront of science

(see chapter 4)

- DIFFER will upgrade its Pilot-PSI facility, which combined with the Ion Beam Facility will enable *in situ* and *operando* studies of materials under extreme conditions in energy systems.



- DIFFER will further develop new facilities capable of *in situ* and *operando* studies, in particular using the Ion Beam Facility for the study of energy systems in general. An NWO Groot proposal will be prepared in close collaboration with DIFFER's research and industrial partners.

Connecting networks of scientific, educational, industrial and societal partners

(see chapter 5)

- The DIFFER PSI and IBF facilities will be positioned as a world-wide leading user facility to study materials under extreme thermal heat and particle flux conditions.

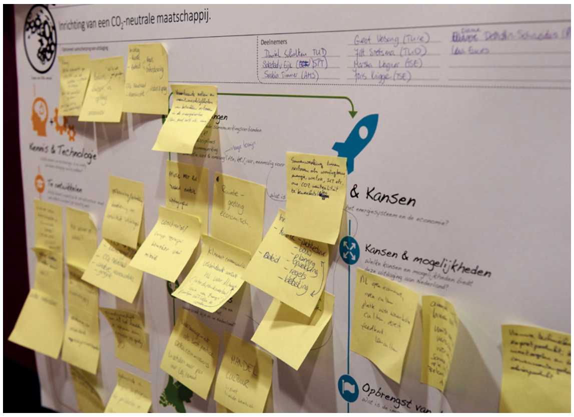
- Together with TU/e, DIFFER will establish a virtual Center for Computational Energy Research (CCER) which will focus on multi-scale computational challenges critical to the understanding of energy systems for a smooth and successful transition towards a sustainable global energy infrastructure. The long-term goal of CCER is to create a highly visible and truly interdisciplinary Dutch hub for computational energy research.

Coordinating energy research in the Netherlands

(see chapter 5)

- DIFFER will continue its organizing and facilitating role to strengthen the energy research community and provide leading input to achieve agenda setting at NERA, the Topsectors and the NWA. DIFFER will initiate a national, goal-oriented program on Electrochemical Conversion and Materials[22,23], strengthening DIFFER's Solar Fuels research in close partnership with the relevant Topsectors and aligned with the challenges as defined in the NWA.

- DIFFER will use its leading and coordinating role (as single Dutch beneficiary for EUROfusion) to develop a national research program on nuclear fusion. This program will be aimed at using the synergy of other world leading facilities in the Netherlands, notably in the fields of material characterization using the ion beam (DIFFER), neutrons (NRG and RID) and positrons (RID).



Ensuring a viable, healthy organization

(see chapter 6)

- DIFFER will aim at a high employability of its senior staff, both inside and outside of DIFFER, to stimulate internal and external job mobility while ensuring the preservation of critical knowledge within the organization.

- DIFFER will offer its employees diversity training programs. Moreover, DIFFER will carry out honest and transparent recruiting procedures for its positions and, in cases of equal qualifications, will favor an increase in the diversity of its workforce.

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[22] The program will include the research on photo- and plasma- assisted electrochemical pathways.

[23] Topsectors Energy, Chemistry and High Tech Systems and Materials have taken the initiative to install a committee for the Dutch Ministry of Economic Affairs to prepare an advice on a long-running, goal-oriented program on Electrochemical Conversion and Materials. The committee is chaired by DIFFER director Prof.M.C.M. van de Sanden.

3 DESCRIPTION OF RESEARCH

The research of DIFFER finds its origin in one of the biggest challenges facing humanity: providing breakthrough solutions to the energy and global warming issue. In the short term the supply of sustainable energy will be primarily in the form of electricity generated by wind and sun. Storage and transport are key issues here, which motivates DIFFER's solar fuels research into renewable electricity driven chemistry, producing chemicals and fuels starting from CO_2, H_2O and N_2. Fusion energy holds an exciting promise to meet the energy challenge, albeit in the longer run. DIFFER's research in this field concerns the challenges of the power exhaust and plasma regimes of operation of nuclear fusion reactors. Common to both themes, DIFFER's expertise and facilities enable a cross-cutting approach where in situ and operando[24] studies in combination with multi-scale modeling and active control hold a promise not only for solar fuels and nuclear fusion but for the broader field of energy research as a whole (see sidebar Cross-cutting approach in Chapter 2).

3.1 Solar Fuels research program

a. Goal and ambition

In the DIFFER Solar Fuels program, photons or electrons are used to drive chemical processes utilizing water (H_2O), carbon dioxide (CO_2) and nitrogen (N_2) as building blocks for the synthesis of fuels and chemicals[25]. Three major chemical pathways can be distinguished here: **water electrolysis and thermo-catalysis**; **electrochemistry**; and **photo-electrochemistry & photo-catalysis**. The scientific and technological challenges of the three pathways define the ambitions of the DIFFER Solar Fuels research program, setting out to tailor and control the chemical reactions from the molecular level to the macro scale.

As becomes apparent from a number of dedicated roadmap studies, each pathway is at a different stage of development, but none is energy and cost efficient yet. For electricity driven chemistry, a roadmap proposed by EASE/EERA provides a useful starting point[26], even though it is largely devoted to non-chemical conversions (such as flywheels, hydrostorage, etc.) and only to a lesser extend describes the route for chemical energy storage. For photon driven chemistry pathways the recent EuChems white paper "Solar driven chemistry" defines the research questions to be addressed[27].

I. Water electrolysis & thermo-catalysis

This pathway starts with the generation of H_2 from H_2O and renewable electricity by means of an electrolyzer, followed by conventional thermo-catalysis based chemical processes (e.g. Fischer-Tropsch to synthesize synthetic hydrocarbons or Haber-Bosch to produce ammonia).

In terms of overall energy efficiency and practical realization this pathway is clearly ahead of the two others. However, successful implementation requires additional research in the fields of

- Materials science (e.g. research into the replacement of robust non-abundant materials such as the electrode materials and catalyst use in PEM electrolyzer);
- Systems engineering (e.g. heat integration with respect to the intermittency aspect of renewable electricity in the thermo-catalysis based chemical processes, but also the aspect of scale).

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[24] The term *"operando"* provides a single word that underlines the simultaneous evaluation/monitoring of both structure (e.g. catalytic active sites and surface reaction intermediates) and activity (e.g. catalytic activity and selectivity).

[25] The use of concentrated solar power to produce hydrogen or carbon monoxide from water and carbon dioxide by means of thermo-chemical processes is not considered here, as well as bio-based approaches.

[26] Technical annex, joint EASE/EERA recommendations for a European Energy Storage technology development roadmap towards 2030 (2013)

[27] Solar driven chemistry, a vision for sustainable chemistry production, EuChems (2016)

These are key research topics to reduce the cost of the produced hydrogen[28] and enable a successful scale-up to the GW level.

II. Electrochemistry

This pathway utilizes renewable electricity to produce chemical and fuels in direct electrochemical processes from CO_2*,* H_2O *and* N_2*, e.g. electrochemical production of ammonia from* H_2O *and* N_2*, or electrochemical reduction of* CO_2 *and* H_2O *to generate hydrocarbons. Combinations of plasma activated processes with electrochemical approaches also are part of this pathway.*

Key challenges here are:

- A fundamental understanding of energy/electron transfer processes at the electrochemical electrolyte-electrode interface;
- Research into the development of robust and earth abundant electro-catalysts with higher selectivity and catalytic activity;
- Novel approaches to overcome the limitation of kinetics and selectivity of key catalytic processes for water splitting, carbon dioxide reduction or activation of nitrogen[29].

III. Photo-electrochemistry & photo-catalysis

This pathway uses photons to reduce for example CO_2 *or to split* H_2O *using photo-catalysts. Other approaches using so called photo-electrochemical cells (PEC) utilize photon induced electrochemical processes to generate chemicals directly from* CO_2*,* H_2O *and* N_2*.*

Important research challenges addressed here are:

- Improvement of photon absorption and charge carrier generation;
- Prevention of charge carrier recombination and improvement of charge transport across the different interfaces in a PEC;
- Development of stable and earth abundant photo-catalysts and photo-electrodes.

In addressing the challenges described above, many global consortia and research groups[30,31] focus strongly on catalysis, in particular on finding robust earth abundant water splitting and CO_2 reducing photo- and electro-catalysts. Applying a combined modelling and combinatorial materials discovery approach, the search is for catalysts with optimal selectivity and activity, and resulting in low overpotentials when used in a (photo-electrochemical) device[32]. It remains a challenge, however, to electrochemically reduce CO_2 (because of its low solubility in water and the cathodic evolution of H_2 as a competing reduction product) and to activate nitrogen (because of the strong covalent bond).

In heterogeneous photo- and electro-catalysis novel approaches are considered imperative to overcome the limitation of kinetics and selectivity of key catalytic processes for water splitting, carbon dioxide reduction, and activation of nitrogen. Many of the energy efficiency limiting processes are present at interfaces, especially at the electrode-electrolyte interface. Improving these interfacial processes is hampered by a lack of understanding of the energy/electron transfer processes that play a key role here. Controlling the structure of interfaces on the nanoscale is a promising research approach which will allow for the optimization of performance and durability of the (photo-)electrode-electrolyte interface[33].

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[28] $1.95/kg production cost based on SMR path: 3.1 Hydrogen Production in "DOE Multi-Year Research, Development, and Demonstration Plan" (2015) http://energy.gov/sites/prod/files/2015/06/f23/fcto_myrdd_production.pdf

[29] A. Vojvodic and J.K. Nørskov, National Science Review **2,** 140 (2015)

[30] J.H. Montoya et al., Nature Materials **16,** 70 (2017)

[31] She et al., Science **355,** 146 (2017)

[32] N. Lewis, Nature Nanotechnology **11,** 1010 (2016)

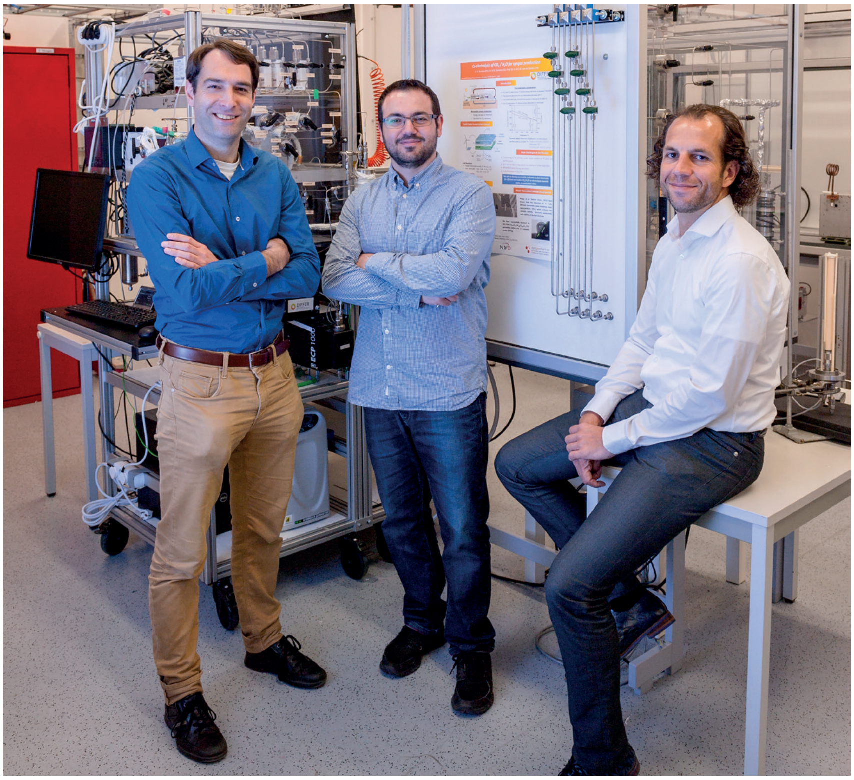
[33] T.S. Irvine et al., Nature Energy **1,** 1 (2016)

Another substantial research effort is aimed at investigating stable and abundantly available novel photo-absorber materials to be used as photo-electrodes in photo-electrochemical cells[34]. The widely used PV grade semiconductors are prone to corrosion and exhibit poor stability in aqueous solutions, which requires strategies for protecting the photo-electrode. Non-PV grade semiconductors, usually metal oxides, have a greater intrinsic stability but display inferior conductivity for holes and electrons. To improve on this, ternary and quaternary metal oxides, oxynitrides, or carbon-based materials are investigated. Common to these approaches, again, is the use of nano- and micro-structuring of materials to improve the photo-absorbing properties, to enlarge the electrode-electrolyte interface, and to improve charge separation by decreasing transport distances.

Approaches in developing integrated devices are based on semiconductor micro- and nano-arrays combined with (polymer) membranes. Strongly developing research topics are novel ceramic proton transporting membrane-based electrochemical reactors that integrate the splitting of water with the hydrogenation of carbon dioxide to methane/methanol, or nitrogen to ammonia[35]. Achieving adequate selectivities and sufficient conversion rates remains, however, a challenge.

b. Research Direction

As mentioned earlier, the starting point for the DIFFER Solar Fuels research is the common challenge of all pathways: to be able to tailor and to control chemical reactions from the molecular level to the macro-scale. To this end it develops **along three research lines** that lie across the three pathways and are crucial and promising in meeting the Solar Fuels challenge. Focusing on these research lines provides DIFFER with an excellent opportunity to contribute to the challenge while taking a distinctive position in the global field of Solar Fuels research. The three research lines reflect the multidisciplinary and programmatic DIFFER approach that uniquely combines fundamental use-inspired research on materials science and engineering; electro-chemistry and catalysis; plasma physics and chemistry; solid state physics; and resonant photonics:



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[34] K. Sivula et al., Nature Reviews Materials **1**, 1 (2016)
[35] Lei Bi et al., Chem. Soc. Rev. **43**, 8255 (2014)

Sidebar 6:
Identifying limiting processes at photo-electrochemical interfaces in water splitting

Photo-electrochemical (PEC) water splitting is a promising future technique to renewably convert sunlight directly into a fuel. However, currently performance and efficiency are still too low. One main reason for this is that the limiting processes at the solid-liquid PEC interface are not identified. At DIFFER, we are developing a new and unique multiscale approach that tackles this challenge by combining experiments with modeling & simulations.

In the experiments, we measure the PEC properties by electrochemical methods including potential and light modulation. In combination with operando *Fourier Transformed Infrared (FTIR) spectroscopy, we can determine the species and intermediates at the solid-liquid interface at different operation points of the PEC cell. This allows us to relate the performance of the PEC cell not only to the structure of the solid electrode, but also to the chemical signature of the interface.*

In parallel, we simulate the same interface by Density Functional Theory (DFT) methods on the atomistic level based on an electrochemical model. Free energy calculations allow for determination of the limiting reaction step and for estimation of the reaction rate constants.

Both experimental FTIR and simulated DFT results feed into a state-space model on continuum level to simulate electrochemical data as measured in the experiments. This approach will enable us to identify the limiting processes at PEC interfaces and - with this knowledge - to design improved interfaces based on better materials and advanced 3D architectures.

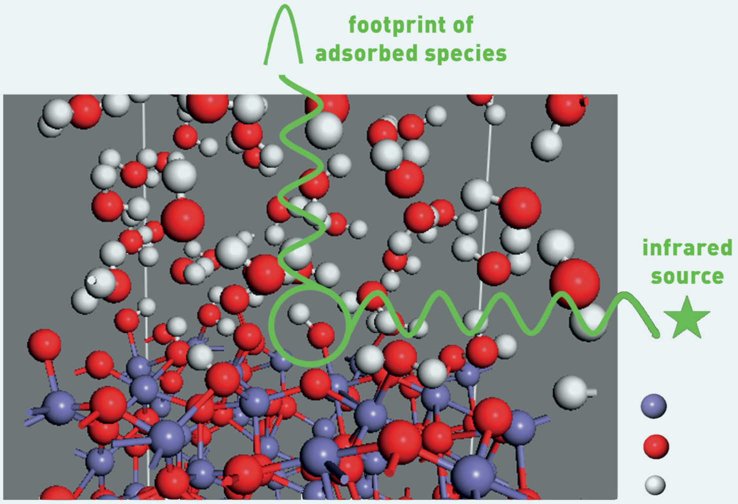
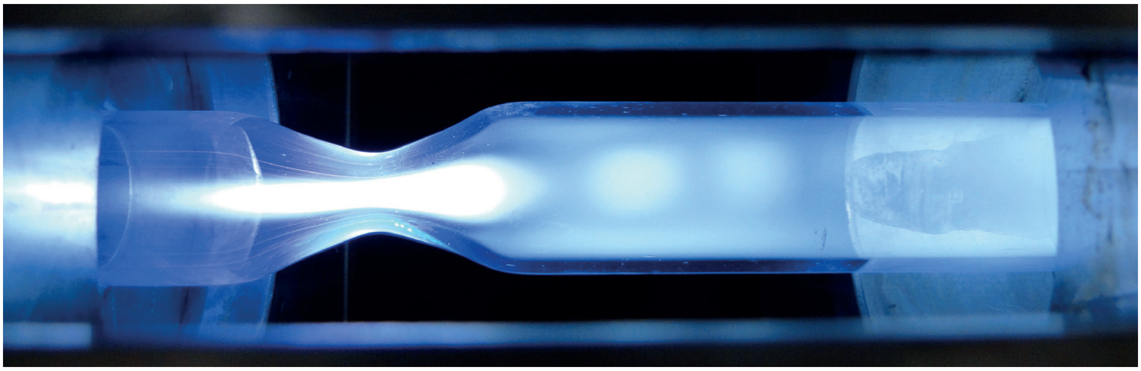


Figure 3.1. Atomistic structure of the iron oxide (photo-electrode) – water (electrolyte) interface in photo-electrochemical water splitting. Surface species and intermediates during the water splitting process are calculated by atomistic modeling and are measured by operando infrared spectroscopy. These results feed into continuum modeling to simulate the electrochemical interface for identifying the limiting processes in experimental interfaces.

I Non-thermal chemical processes

Research groups: NFC, PSFD, MSS, CEPEA, CPPC

This research line explores novel concepts, using plasma and radiation to induce non-thermal phenomena to control and tailor chemical conversion reactions. These (often strongly out-of-equilibrium) processes provide a new approach to overcome the limitation of kinetics and selectivity of key catalytic processes for water splitting, carbon dioxide reduction or activation of nitrogen. This research will open new opportunities to achieve both high energy efficiencies - exceeding purely thermal equilibrium values - and high product selectivity, all at reduced temperature. Two examples of unique fundamental approaches addressed at DIFFER are the use of non-equilibrium plasma, which builds on key results from the field of mode selective chemistry[36], and plasmon assisted catalysis using nanostructured materials[37], both exploiting the prevalent non-thermal effects.



II Functional materials and interfaces

Research groups: APPFF, CEPEA, EMI, MSS, NEA, PFE, SSE

This research line focuses on the development, characterization and utilization of novel materials for chemical conversion, storage, and separation. Surfaces and interfaces are crucial to the performance and durability of the (photo-)electrochemical cell. Their properties dictate performance in the case of product transport, separation, and solid-state storage/release systems. Enhancing the functionality of such systems requires control and manipulation of materials properties across length scales, from formation and characterization on the nanoscale to reproducible production of industrial scale quantities. For instance, the structure-property relation of functional materials used as electrodes in contact with the electrolyte in (photo-) electrochemical cells is poorly understood, as are the processes taking place at these interfaces[38].

Studying the multi-scale processes *in situ* and *operando* in (photo-)electrochemical cells, supported by multi-scale computer simulations using physics model based approaches, will provide novel pathways to develop functional materials that improve the activity and performance of the electrochemical interface (e.g. interfacial energy/electron transfer and prevention of charge recombination[39]). In a similar way breakthrough solutions can be achieved for energy storage on the nanoscale[40] and for the development of advanced functional films (e.g. as ionic conducting membranes for electrochemical applications)[41].

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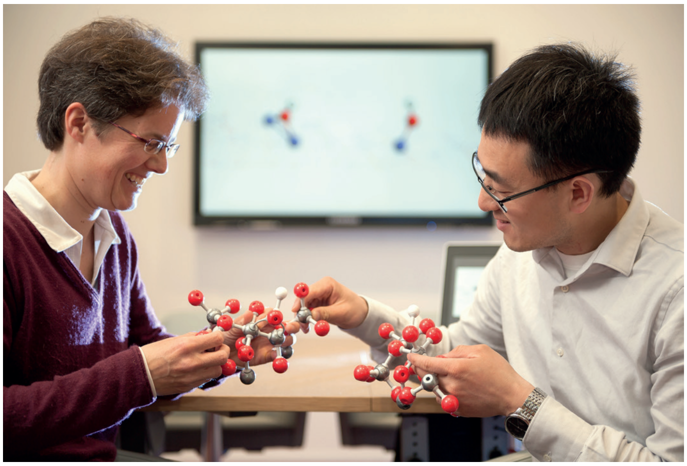
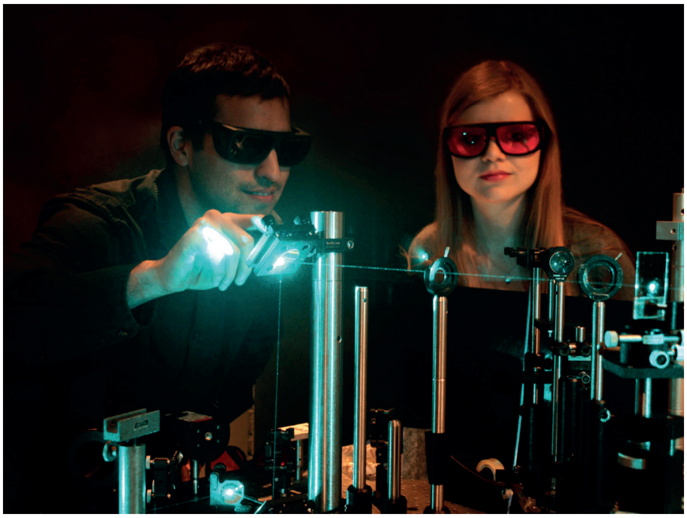
[36] F. Fleming Crim, PNAS **105** 12654 (2008); P. Maroni et al., Phys. Rev. Lett. **94**, 246104 (2005); S. Yan et al., Science **316**, 1723 (2007)
[37] D.F. Swearer et al., PNAS **113** 8916 (2016); A. Marimuthu et al., Science **339**, 1590 (2013)
[38] K. Sivula et al., Nature Rev. Mater. **1**, 1 (2016); J.H. Montoya et al., Nature Mater. 16 70 (2017); She et al., Science **355**, 146 (2017)
[39] X.-Q. Zhang, A. Bieberle-Hütter, ChemSusChem **9**, 1223 (2016)
[40] T.C. Narayan, F. Hayee, A. Baldi et al., Nature Comm. **8**, 14020 (2017); T.C. Narayan, A. Baldi et al., Nature Mater. **15**, 768 (2016); A. Baldi, T. C. Narayan et al., Nature Materials **13**, 1143 (2014)
[41] J.T.S. Irvine et al., Nature Energy **1**, 1 (2016)



III Light-matter interaction

Research groups: CEPEA, EMI, NEA, PFE, SSE

The interaction of light with matter gives rise to a wide range of phenomena that can be used to convert electromagnetic energy into chemicals and to control and tailor chemical reactions. We will exploit nano-photonic concepts such as deep sub-wavelength phenomena and light-matter interaction at the nanoscale to tailor (photo-)chemical reactions at a molecular level. The use of open cavity structures or nanostructured functional materials can improve light absorption for a better overall efficiency of (photo-)electrochemical cells through tailoring the spatial distribution of photo-generated electron-hole pairs, minimizing the charge recombination[42]. Also light-matter interaction can be enhanced to reach the strong coupling limit. This is a new research field termed Cavity Enhanced Chemistry[43], in which material properties can be reversibly modified, enabling an improved charge transport and new chemical reaction paths.



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[42] M. Ramezani et al., Optica **4,** 31 (2017)

[43] T.W. Ebbesen, Acc. Chem. Res. **49,** 2403 (2016)

Sidebar 7: Nano-photonic operando *study of chemical reactions*

Nanotechnology allows unprecedented control over the properties of functional materials used as catalysts and photo(electro)catalysts in a wide range of chemical reactions. DIFFER exploits nanoscale light-matter interaction on metal nanoparticles to enhance solar-to-fuel conversion and to detect key reaction intermediates in photo(electro)chemical processes such as H_2O *oxidation and* CO_2 *reduction.*

A key feature of nanostructured materials is their size-tunable properties. Studies in which the properties of nanomaterials are characterized in ensemble are however limited by the sample inhomogeneity and can only return an average picture. Scientists therefore need to develop methods to characterize functional nanomaterials both at the single particle level and in operando *conditions. At DIFFER we tackle this challenge by exploiting the resonant interaction of individual nanoparticles with light, to probe and control their* in situ *response.*

In our studies of metal nanoparticles, we use their strong scattering and absorption of light due to the excitation of plasmon resonances. These collective oscillations of free electrons can influence chemical reactions by inducing strongly localized electromagnetic fields, exciting non-equilibrium charge carriers, and heating the nanoparticle surface. In our research, we study these processes using single particle optical methods, such as super-resolution localization microscopy and dark-field scattering spectroscopy. Our approach allows simultaneous control over material properties as well as over irradiation characteristics, and a direct comparison of experimental results with predictions from theory and numerical modelling.

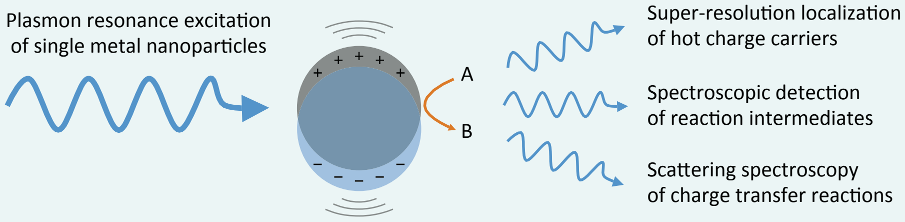

Figure 3.2. Single-particle methods to study chemical reactions at the nanoscale.

c. Planning

This Strategic Plan comes at an important phase in the transition of DIFFER. During the past years a viable Solar Fuels research workforce was established, and the years 2017-2021 will demonstrate its power to contribute to the field. To further strengthen the Solar Fuels research, DIFFER will initiate a national, goal-oriented program on Electrochemical Conversion and Materials. This will be undertaken in close partnership with the relevant Topsectors and aligned with the challenges as defined in the NWA. To strengthen DIFFER's position in the field of multi-scale modeling, DIFFER will establish together with TU/e a virtual Center for Computational Energy Research (CCER) which will focus on multi-scale computational challenges that are relevant to both the Solar Fuels and Fusion Energy research (see section 3.3).

d. Personnel

The research is realized by eight research groups, a DIFFER-Fujifilm group and a joint DIFFER-TU/e group. Collectively, these groups combine expertise in catalysis, photo-, and electrochemistry, plasma physics and chemistry, nano-photonics, solid state physics, surface chemistry and computational modelling.

Theme Solar Fuels

Atmospheric Plasma Processing of Functional Films
Dr. Hindrik de Vries

Catalytic and Electrochemical Processes for Energy Applications
Dr. Mihalis Tsampas

Computational Plasma Physics and Chemistry
Dr. Paola Diomede

Electrochemical Materials and Interfaces
Dr. Anja Bieberle

Materials and Surface Science
Dr. Michael Gleeson

Nanomaterials for Energy Applications
Dr. Andrea Baldi

Nonequilibrium Fuel Conversion
Dr. Gerard van Rooij

Photonics for Energy
Prof. Jaime Goméz Rivas

Plasma Solar Fuel Devices
Dr. Waldo Bongers

Solar Fuels Facilities & Instrumentation
Dr. Stefan Welzel

Storing Solar Energy (DIFFER - TU/e)
Prof. René Janssen

APPFF - Investigating atmospheric plasma processes for large scale synthesis of advanced functional thin films for CO_2-neutral solutions.

CEPEA - Combining solid state electrochemistry with (photo)catalysis to improve the efficiency of existing and to develop new routes for energy storage.

CPPC - Development of models for molecular plasmas dynamics and chemical kinetics.

EMI - Understanding and tuning the properties of electrochemical materials and interfaces to reach the highest performance and to supply alternative, sustainable energy solutions for the future.

MSS - Getting fundamental insights into chemical and physical processes occurring during the interaction of solar fuel relevant molecules with materials.

NEA - Exploring fundamental challenges and application opportunities of nanomaterials for energy conversion and storage.

NFC - Understanding of plasma chemical dissociation of CO_2 for the development of a generic plasma chemical route as the first step in CO_2-neutral fuel production.

PFE - Investigating light-matter interaction in a broad range of frequencies to contribute to energy conversion.

PSFD - Gaining efficient production of high energy density fuels or intermediates such as carbon monoxide and hydrogen gas by plasma assisted conversion.

SFFI - Facilitating all solar fuels research groups at DIFFER by reconstruction of labs and developing, operating and maintaining all unique devices and diagnostics.

Molecular Materials and Nanosystems, (Prof. René Janssen, TU/e-M2N). To design, develop, and investigate organic, polymer, and hybrid semiconductors integrated in novel opto-electronic devices for energy conversion and storage.

Membrane Materials and Processes, (Prof. Kitty Nijmeijer, TU/e-MMP). Tailoring membrane chemistry and morphology to control mass transport in macroscopic applications and combine and integrate material science and process technology.

3.2 Fusion Energy research program

a. Goal and ambition

The Fusion Energy research program contributes to the development of practically inexhaustible, clean power generation through the thermonuclear reaction of hydrogen isotopes deuterium and tritium. A nuclear fusion reactor provides a concentrated and non-intermittent power source, producing clean, CO_2-neutral energy using practically limitless fuel sources. It can complement distributed sustainableenergy sources to create robust and secure future energy systems.

The global endeavor of constructing ITER will result in the first reactor capable of creating and controlling a ‘burning’ plasma where the power generated by the nuclear fusion reactions will substantially exceed the external input power ($P_{fusion}/P_{in} \geq 10$). After that the European nuclear fusion program EUROfusion aims to realize a demonstration reactor, DEMO, to be operational around 2050.

The goal of the DIFFER Fusion Energy research is to enable the development and validation of science and technology for the design and operation of ITER and DEMO. The primary focus here is on one of the most critical aspects of nuclear fusion energy: the exhaust of heat and particles at the divertor[44]. We develop novel divertor materials solutions, model based plasma controllers, and innovative sensors and diagnostics for the plasma periphery. This requires a fundamental physics based analysis of the radiative peripheral plasma, including impurity migration, detachment and H-mode physics, in co-development with control oriented models and controllers, and new materials.

b. Research directions

DIFFER’s multi-disciplinary and programmatic approach combines use-inspired fundamental research in the fields of materials engineering and science, plasma physics and chemistry, systems identification and integration, and control engineering. The research benefits from the unique facilities for plasma surface interactions (PSI - see chapter 4). The Magnum-PSI facility exposes materials to the extreme conditions (heat and particle loading) of an operational tokamak nuclear fusion reactor, positioning DIFFER as the only institute in the world able to investigate materials for future use in the ITER and DEMO divertors. Combined with other experimental PSI facilities, a sophisticated diagnostic park for plasma and materials characterization, and a substantial modeling effort, DIFFER is capable of detailed studies of a wide variety of plasma surface interaction processes.

In addition, we apply and (co-)develop state of the art physics and control oriented codes for transport, plasma stability, wave propagation and exhaust to design and analyze optimized plasma regimes of operation.

DIFFER’s Fusion Energy research is carried along two major research lines:

I Understanding and control of plasma exhaust

Research groups: CPPC, FFI, IMM, IMT, PEPD

The main aspect of the exhaust challenge is to minimize the flow of heat and particles to the reactor walls, in order to minimize damage. The plasma exhaust is a complex research topic in which fluxes of heat and particles result in a strong coupling of various regions of the plasma: the reactor materials, the plasma sheath, the scrape-off layer and the detachment front, the H-mode barrier and pedestal, and even the plasma core.

The focus of this research line is to unravel the multitude of non-linear interactions in and between these regions. This has both experimental and modeling aspects. The experiments will be carried out in Magnum-PSI and in the European mid-sized tokamaks ASDEX Upgrade and TCV. The modeling effort aims both at the fundamental physics understanding and at control oriented modeling and controller synthesis.

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[44] Roadmap to the Realisation of Fusion Energy, https://www.euro-fusion.org/eurofusion/the-road-to-fusion-electricity/

The research combines fundamental physics studies such as the influence of secondary electron emission on the plasma sheath (the transition layer between the plasma and the solid material target) properties during detachment conditions, H-mode modeling of the migration of atomic and molecular neutrals from the target to the upstream plasma, as well as establishing the role of the exhaust actuators such as the divertor magnetic geometry (flux expansion and its derivative) and the impurity seeding.

Sidebar 8: Multi-spectral imaging of tokamak edge and divertor plasmas

Future large-scale tokamak reactors will require a large fraction of the nuclear fusion power to be radiated away, in order to achieve a plasma state in which the energy and particle fluxes are largely decoupled from the machine walls, so called plasma detachment. Fast, spectrally resolved imaging provides detailed quantitative information about the detachment process. The PEPD group is developing the MANTIS diagnostic (Multi-spectrally Acquiring Narrowband Time-resolved Imaging System) which aims to provide all the benefits of imaging, while also capturing sufficient spectral information to enable a quantitative determination of key plasma parameters (e.g. temperature, density) in the whole divertor region at once. The MANTIS diagnostic features an optical cavity consisting of concave spherical mirrors, relay lenses, and narrow-band filters, re-imaging the plasma up to ten times. The filters pass a narrow wavelength band around a chosen spectral line and act as a mirror for the rest of the visible spectrum. The passed light is imaged onto a camera sensor, while the reflected light continues towards the next channel. The MANTIS diagnostic will be applied to both the TCV tokamak and our in-house linear device Magnum-PSI. The objective is to not only generate new insights into the physics and chemistry of detachment, but also to enable new active feedback control strategies based on 2D sensor data at high time resolution.

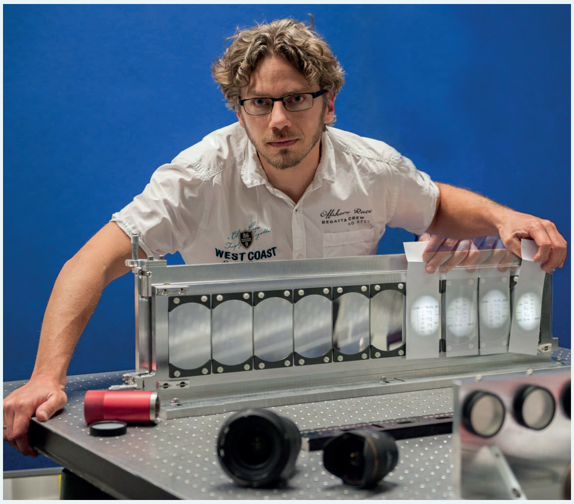

Figure 3.3. The MANTIS diagnostic employs a setup of ten cameras behind ten narrow-band filters to simultaneously image the 2D distribution of ten emission lines in the divertor region.

Combining real-time measurements and physics based models for the development and validation of real-time control strategies is vital in view of the migration of our controllers from present-day devices to future tokamaks such as ITER and DEMO and to ensure the optimized regime of plasma operation.

A key concept is that of the state observer, a dynamic model of the plasma that is evaluated in real-time. The state observer can be used to provide optimal real-time estimates of the plasma evolution. As nuclear fusion power plants will run a very limited number of scenarios, it is viable to apply a model based approach. In particular, the ability to sense plasma parameters will be substantially reduced in comparison to ITER and present day tokamaks. Hence, the use of state observers is expected to be vital to optimally estimate the plasma state, perform faster than real-time predictions and to evaluate in real time the optimal discharge and actuator trajectories, and issue early warning if the discharge is deviating from the reference. The development and testing of such techniques are in the core of our program.

The expertise of DIFFER in the field of control is also of relevance to fields other than nuclear fusion energy, which offers opportunities for cooperation. Elements of the plasma control problem that are of particular interest for the control community are the sharing of actuators for control tasks, the limited sensorsina nuclear fusion reactor, the operation in the vicinity of operational limits, and the fact that the system is distributed. DIFFER actively pursues valorization of its knowledge regarding these important control issues.

II Research and engineering of materials under extreme conditions

Research groups: CPPC, FFI, PMI

The conditions in a nuclear fusion reactor are so extreme that dedicated materials for the plasma facing components need to be developed and validated. The experimental materials research facilities at DIFFER are uniquely placed for such research since ITER and DEMO relevant fluxes and fluences can be obtained under well diagnosed conditions. Adding to this, controlled exposure experiments can be combined with measurement of structural changes using a variety of in-situ characterization techniques (see next chapter). To meet the challenge of obtaining a thorough fundamental understanding of the mechanical and functional performance of the materials in relation to their microstructure, the experimental results obtained at DIFFER’s PSI facilities are complemented with multi-scale structure-property modeling in collaboration with TU/e (Dr. J.A.W van Dommelen) and SCK•CEN Mol (Dr. D. Terentyev).

A key focus is on the tungsten used for the divertor plates in ITER, where it is imperative to establish how the production of the tungsten as well as the manufacturing of tungsten components will affect the orientation, size and shape of the grains and grain boundaries and the possible presence of voids and/or dispersoids.

DIFFER plays an important role in the divertor concept improvement as well as the validation chain for nuclear fusion reactor components. With TU/e and the German SME Research Instruments we participate in the M2i program on this urgent ITER relevant program. As Research Instruments obtained a contract to build prototypes for the ITER vertical divertor targets, the M2i program opens the opportunity to test and validate the materials, improve the design, and to test and validate the design on WEST. DIFFER already worked with the medium sized tokamak WEST (CEA) on W erosion (Dr. Gerard van Rooij) and studies of the plasmas sheath (Dr. Hennie van der Meiden), and this program will intensify the collaboration with the WEST team.

Sidebar 9: Real-time capable first principle transport modelling for tokamak prediction and control

The primary mechanism constraining plasma confinement in tokamaks, and hence the nuclear fusion power, is turbulence. Predicting and controlling turbulent energy transport is a grand challenge in nuclear fusion science. Recent significant progress in direct numerical simulation with nonlinear gyrokinetics now routinely reproduces experimentally measured transport fluxes in many regimes. However, these computationally expensive models are intractable for full tokamak discharge simulations. For real-time control applications, a 12 order of magnitude calculation speedup is required. Quasilinear transport models co-developed at DIFFER have achieved significant predictive success while being 6 orders of magnitude faster than nonlinear simulations, allowing for more routine predictions and validation of the underlying theory. However, real-time applications are still not feasible.

At DIFFER, we explore a new approach to speed up transport model calculations towards real-time, without reducing the physics fidelity. The crux of this work is the emulation of existing tokamak quasilinear turbulent transport models via neural network regression of compiled model output databases. Applying these techniques for tokamak transport modelling is unprecedented, and opens up a myriad of possibilities such as efficient offline discharge optimization and real-time scenario trajectory optimization and control. We apply the new transport models within the real-time capable RAPTOR tokamak simulator (developed by our partner TU/e)[45], a leading control-oriented simulation suite. Ultimately, by generalizing this technique to additional physics components, we aim towards high fidelity real-time entire device simulation, a prerequisite for the operation of future nuclear fusion reactors.

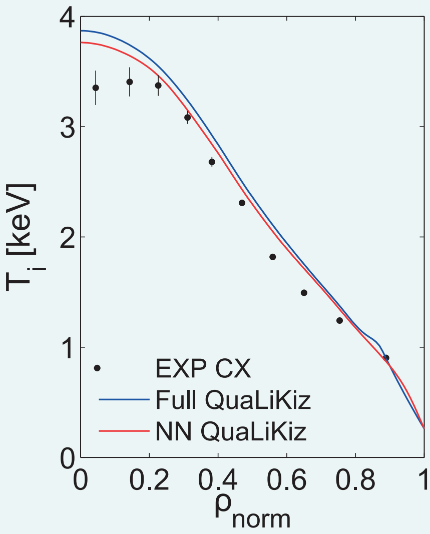

Figure 3.4. Comparison of JET tokamak ion temperature radial profile measurements (discrete points) to quasilinear turbulence model predictions using the full QuaLiKiz model[46] (blue curve) and a neural network emulation of QuaLiKiz (red curve). The neural network model calculates a radial profile of turbulent transport fluxes within 1ms, while still maintaining high physics fidelity.

Alternatively, for DEMO the use of liquid metals is proposed to shield the plasma facing components. This could overcome several of the limitations of solid materials under extreme nuclear fusion loads and opens the possibility for additional heat removal (beyond conduction). PSI studies at DIFFER will give insight in the effects of plasma-liquid interactions such as corrosion, evaporation, wetting and chemical reactions as well as vapor shielding. In collaboration with Princeton Plasma Physics Laboratories an enclosed lithium vapor shielding divertor concept will be tested in Magnum PSI in 2018.

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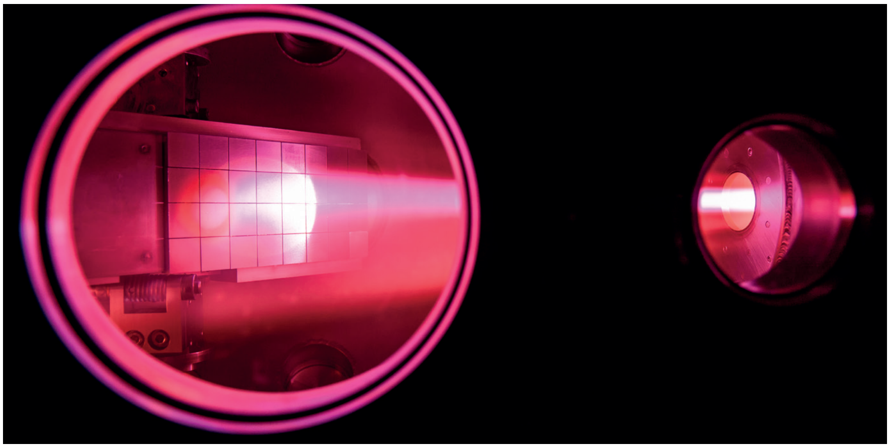
[45] F. Felici and O. Sauter, Plasma Phys. Control. Fusion **54**, 025002 (2012)
[46] C. Bourdelle, J.Citrin et al., Plasma Phys. Control. Fusion **58**, 014036 (2016)



DIFFER's expertise and facilities in the field of materials under extreme conditions is also very relevant to many fields other than nuclear fusion. Here opportunities arise for long term collaborations. A striking example is in the field of advanced lithography, where ASML company has expressed interest to use DIFFER facilities to study plasma-material interactions of hydrogen plasmas and high density tin plasmas. With the Technical University of Delft, NRG and ECN, aspects of additive manufacturing and welding of nuclear fission and fusion reactor relevant materials are investigated.

An interesting cross-over is the development of a system for Collective Thomson Scattering that enables unambiguous localized measurement of ion temperature, velocity and impurity concentration of the near-surface plasma in Magnum-PSI as well as that of welding arcs. This will seriously improve the modeling and understanding of plasma-wall interaction.

c. Planning

The EUROfusion roadmap leads the way in developing the DIFFER nuclear fusion research portfolio. For the coming years two major programs are in place through EUROfusion (Horizon 2020) funding:

- FOM program 'Taming the Flame' (FOM Program 171, 2016 - 2021);
- M2i-program 'Materials Behavior under extreme particle and radiation loading' (2016 - 2020).

These programs ensure the financial viability of the DIFFER Fusion Energy research throughout the better part of the 2017-2021 period covered by this strategic plan. FP 148 provided the matching for the ongoing Impulse program on materials in extreme conditions, established with TU/e.

To follow-up on these programs, initiatives are underway to establish a national Dutch nuclear fusion program around the themes of materials, plasma periphery and control and diagnostics. This would enable DIFFER and partners to provide key contributions to the power exhaust challenge of nuclear fusion reactors. This consortium will also be in an excellent position to initiate a research program on materials under extreme conditions towards other, non-nuclear fusion (energy) systems.

To further strengthen DIFFER's position in the field of control, DIFFER will establish a new research group on control engineering and systems identification for energy systems. The group will work in close partnership with the Eindhoven University of Technology faculties of Mechanical Engineering and Electrical Engineering and the world leading systems identification laboratory of the Vrije Universiteit Brussel. The focus of this group will be the development and application of methods for identifying the distributed transport of heat and particles in energy systems. The group has already established links with the medium sized tokamaks ASDEX Upgrade and TCV, and the Japanese stellarator LHD, and will also closely collaborate with the new stellarator Wendelstein 7X.

DIFFER strengthened collaboration with the TU/e in the field of multi-scale modeling by establishing the virtual Center for Computational Energy Research (CCER), which will focus on multi-scale computational challenges that are relevant to both the Fusion Energy and Solar Fuels research.

d. Personnel

Six Fusion Energy research groups combine expertise in modeling of the plasma core and periphery; instrumentation; plasma surface interaction; and the development and operation of the plasma-wall interaction facilities. The group structure reflects the programmatic and integrated approach of the nuclear fusion program:

Theme Fusion Energy

Computational Plasma Physics and Chemistry
Dr. Paola Diomede

Fusion Facilities & Instrumentation
Dr. Hans van Eck

Integrated Modelling and MHD
Dr. Egbert Westerhof

Integrated Modelling and Transport
Dr. Jonathan Citrin

Plasma Edge Physics and Diagnostics
Dr. Ivo Classen

Plasma Material Interactions
Dr. Thomas Morgan

CPPC - Development of models for molecular plasmas dynamics and chemical kinetics.

FFI - Maintains and extends the key experimental assets of the DIFFER Fusion Energy program: the Plasma Surface Interaction facilities.

IMM - Focused on plasma core MHD instabilities and Electron Cyclotron waves to stabilize them. The group will develop towards edge MHD instabilities and the modeling of the plasma exhaust.

IMT - Carries out first-principle-based predictions of turbulent plasma transport, including fundamental studies with high-performance-computing nonlinear codes, development of reduced quasilinear turbulent transport models and control-oriented emulations.

PEPD - Design of state-of-the-art diagnostics and sensors.

PMI - Investigates the science of plasma wall interaction.

3.3 Opportunities for new program development

After attracting excellent scientists, and establishing its unique research facilities and computational center, DIFFER will pursue opportunities to extend its research portfolio to materials for additional energy systems.

a. Goal and ambition

Although DIFFER's research is primarily organized around the two themes discussed above, cross-fertilization and collaboration is very important at DIFFER. Adding to this, the unique DIFFER infrastructure for research into materials and interfaces is instrumental in establishing a common perspective. An opportunity for the DIFFER Solar Fuels research is to benefit from knowledge and expertise developed in the Fusion Energy research. For instance system identification methods already prove relevant to model complex advanced electrochemical processes. Furthermore the Upgraded Pilot-PSI and nano-PSI systems will be employed for nano- and micro-structuring of (photo-)electrodes for efficient water splitting or carbon capture materials.

The DIFFER approach (described in more detail in the box Cross-cutting approach in Chapter 2) also holds a great promise for energy research beyond Solar Fuels and Fusion Energy. Examples are research into redox flow batteries, metal air batteries, or CO_2 air capture, since they line up with the expertises present and approaches developed within DIFFER. DIFFER therefore stimulates explorative research projects at the fringes of group research, combining the expertise of multiple groups.

In line with these developments is the DIFFER initiative to join a consortium of Reactor Institute Delft and NRG. This consortium is preparing a research program on a Gen IV fission approach, the so-called molten salt loop in a thorium reactor. DIFFER is uniquely placed to participate in the materials research for this program, and could focus on the study of possible synergetic effects of corrosion and radiation induced damages in the materials.

b. Planning

DIFFER will direct resources to explore fundamental research challenges outside the research focus of fusion energy and solar fuels, in order to diversify the research portfolio and be able to incorporate novel developments in energy storage and conversion. Annually a significant fraction of the strategic DIFFER research budget will be set apart for these explorative projects. It can be considered 'seeding' money since successful exploration will lead to new funding opportunities and ultimately the establishment of new research groups. To establish new funding opportunities in line with DIFFER's research outlook, the institute will actively participate in shaping Dutch research policy and the establishment of relevant funding instruments.

c. Personnel

Explorative projects will be carried out by PhD students or postdoc researchers funded through the DIFFER exploratory budget and supervised by PI's from the Solar Fuels and/or Fusion Energy research groups. When successful (demonstrated by the acquisition of additional research funding) this will lead to the employment of more researchers and ultimately to the establishment of new research groups focusing on new research subjects.

Sidebar 10: A virtual center on computational energy research

Together with TU/e, DIFFER initiated a Center for Computational Energy Research (CCER) which focuses on multi-scale computational challenges critical to a smooth and successful transition towards a sustainable global energy system. The CCER will greatly strengthen the fundamental energy research at DIFFER and the TU/e Strategic Area Energy (SAE). Housed at DIFFER, the CCER aims to realize optimum synergy between DIFFER and TU/e by creating a collaborative environment for mutual learning and exchange of ideas. The long-term goal of CCER is to create a highly visible and truly interdisciplinary Dutch hub for computational energy research.

In order to create an environment that is most likely to evoke breakthroughs, the research program is organized according to the scales at which these subjects are treated. This has led to the following research lines:

- *Continuum media & processes*
- *Media & processes at the mesoscale*
- *Materials & processes at the nanoscale*
- *Bridging length & time scales*
- *Computational discovery & machine learning*

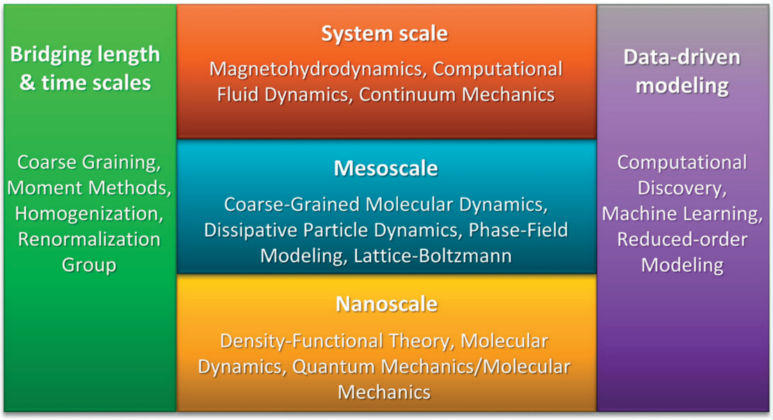


Figure 3.5. Structure of the proposed research program of the CCER, with five different research lines based on scales and their bridging. Typical methods to be used are indicated.

4 RESEARCH INFRASTRUCTURE AND SUPPORT

DIFFER anchors its strong position in energy science through the in-house development and exploitation of a unique and comprehensive high tech infrastructure. In addition to the relevance of this infrastructure for DIFFER's own Fusion Energy and Solar Fuels research themes, a strategic choice of the institute is to develop mid-sized facilities that provide focus and continuity to the international energy research community, and enable DIFFER to bridge the gap between fundamental research and industrial application. Complementing the mid-size facilities at DIFFER are clusters of well-equipped laboratories and an arsenal of dedicated code parks for simulation and modelling. This chapter describes the relevant facilities, setups, modelling capabilities, technical support and human research management in more detail and presents the institute's strategy to ensure that this infrastructure, maintains its top position in global fundamental energy research.

4.1 PSI-lab: Plasma Surface Interaction Laboratory

Part of the DIFFER expertise is centered around the understanding of the interaction between intense plasmas and solid and liquid materials: the research field of Plasma Surface Interaction (PSI). This field is of high and increasing importance in the development of nuclear fusion. At the exhaust of a nuclear fusion reactor, the extremely high heat and particle fluxes push the wall material far from equilibrium, eroding the surface and implanting large numbers of ions into the near-surface region. The unique research facilities of the PSI labs guarantees DIFFER's worldwide impact in the high-priority research area of finding suitable wall designs for nuclear fusion reactors.

	Nano-PSI	**Upgraded Pilot-PSI**	**Magnum-PSI**	**ITER divertor**
n_e [m^{-3}]	$10^{16} – 10^{17}$	$10^{18} – 10^{20}$	$10^{19} – 10^{21}$	$10^{19} – 10^{21}$
T_e [eV]	0.1 – 0.3	0.1 – 2	0.1 – 10	0.1 – 50
Γ_i [m^{-2} s^{-1}]	$10^{19} – 10^{20}$	$10^{22} – 10^{24}$	$10^{23} – 10^{25}$	$10^{24} – 10^{25}$
p_n [Pa]	10 – 100	5 – 20	0.1 – 10	1 – 10
d [mm]	20 - 50	10 – 20	10 - 15	-
B [T]	-	0.2	2.5	~ 5
P_{fd} [MW m^{-2}]	0.0003	5	> 10	> 10
P_{fd} tr. [GW m^{-2}]	-	0.5	2	2 – 4
pulse length [s]	continuous	continuous	continuous	500s
Ion beam analysis	*ex situ*	*operando*	*in situ*	-

Table 4.1 - Plasma parameters in front of the target of the DIFFER PSI devices compared to the ITER divertor strike zones: n_e - electron density, T_e - electron temperature, Γ_i - ion flux density, p_n - neutral pressure, d - plasma diameter, B - magnetic field, P_{fd} - energy flux density, P_{fd} tr. - transient energy flux density (during ms pulse).

Magnum-PSI

DIFFER's flagship experiment is the linear plasma generator Magnum-PSI. This world-class facility is the only machine in the world capable of reproducing the heat and particle loading expected in the divertor region of future nuclear fusion reactors such as ITER and DEMO (see Table 4.1). Magnum-PSI is equipped with a superconducting magnet to provide constant magnetic fields up to 2.5 T, which enables extremely high cumulative plasma fluences for testing of wall materials. Utilizing a specialized wall stabilized arc plasma source, extremely high ion fluxes (> 10^{24} m^{-2} s^{-1}) with heat fluxes of up to 50 MW m^{-2}, can be achieved in steady state operation. A dedicated pulsed power supply is developed to investigate the effect of sudden energy eruptions from the nuclear fusion plasma (e.g. Edge Localized Modes) on the reactor wall materials, where heat loads up to 1 GW m^{-2} can be realized.

Magnum-PSI has been designed to provide excellent optical access and has a large diagnostic suite, giving an extremely well defined set of plasma parameters and information on the retention of fuel species in the exposed material. The system is capable of handling large targets, up to an area of 0.12x0.6 m^2 and weight of 100 kg. The target holder is highly flexible and can be tilted to very low angles (<3°), replicating the incidence angles of plasma onto the target material. These targets can be transported to the material analysis chamber without breaking vacuum to perform *in situ* ion beam analysis for extensive material characterization.

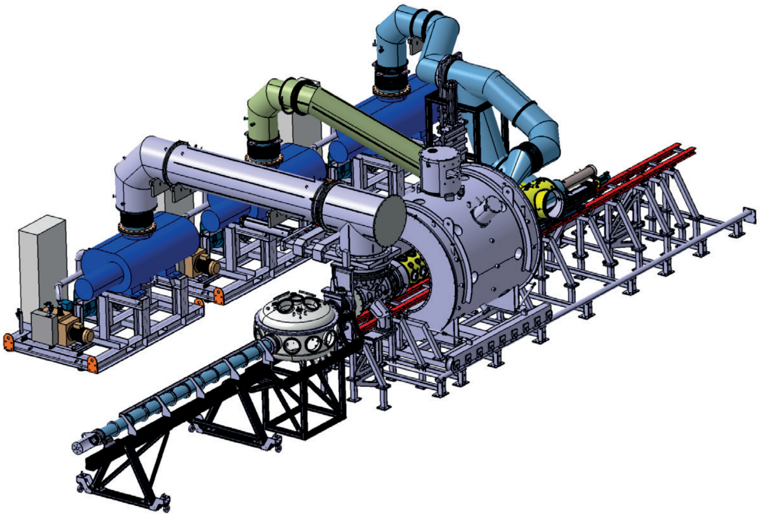


Figure 4.1. Magnum-PSI facility

A key aspect of this work is the development of state of the art diagnostics that enable new investigations. The novel MANTIS multi-spectral imaging diagnostic system presently being developed at DIFFER enables the precise determination of the temperature and migration of impurities in the edge of nuclear fusion plasmas. This will provide information on the profiles of plasma parameters such as temperature and density, and on the physical and chemical processes in the scrape-off layer. It will also enable thorough evaluation of candidate elements to facilitate plasma detachment through impurity seeding, such as Ar, Sn, and W. MANTIS is conceived as a sensor for real-time impurity injection control experiments.

A tangential Thomson scattering system at the ASDEX Upgrade tokamak will provide data regarding electron density and electron temperature, and hence help to determine the distribution of the electron pressure, as well as the current density distribution in the H-mode pedestal. This will prove to be essential input to the development of edge MHD stability codes, with the view to studying Edge Localized Modes.

At Magnum-PSI a new system for collective Thomson scattering is being developed that will allow the study of heavy, cold ions. Combined with incoherent Thomson scattering optimized to study the plasma, this will provide a complete measurement of both the ion and electron distributions.

With its excellent parameter range and diagnostic access, the Magnum-PSI facility is uniquely capable of investigating the evolution of materials during long and intense plasma exposures, especially relevant for lifetime studies of candidate wall materials under extreme conditions.

Sidebar 11:
Collective Thomson scattering for advanced plasma diagnosis in Magnum-PSI

To provide a full picture of the near-surface plasma, Magnum-PSI is equipped with an incoherent Thomson scattering system for electron density (n_e) and electron temperature (T_e) measurements. A novel collective Thomson scattering (CTS) system is now being developed for unambiguous localized measurement of temperature, velocity and impurity concentration of the plasma ions. This will give detailed insight into the properties of the plasma ions as they interact with wall materials.

The extremely high n_e and low T_e (and resulting small Debye length) of the plasma in Magnum-PSI enables application of CTS at relatively short laser wavelengths, as demonstrated for the first time at Pilot-PSI[47] *. In applying CTS to study ITER divertor relevant conditions, the system should be capable of measuring at densities as low as $n_e \sim 5 \times 10^{20}$ m^{-3} and at ion temperatures as low as $T_i \sim 1$ eV. To yield sufficient signal and resolution for the CTS system, a multi-pass laser system enhancing the signal levels with a factor 15 is being developed. A grating upgrade of the spectrometer is in place to improve the spectral resolution from 0.017 nm to below 0.005 nm (at 1064 nm), which, along with developments to minimize stray light, is key to resolving the narrow ion feature spectrum. In all the CTS system enables the measurement of ion temperatures (T_i), impurity concentrations and plasma velocities of the near surface plasma with a spatial resolution of <2 mm.*

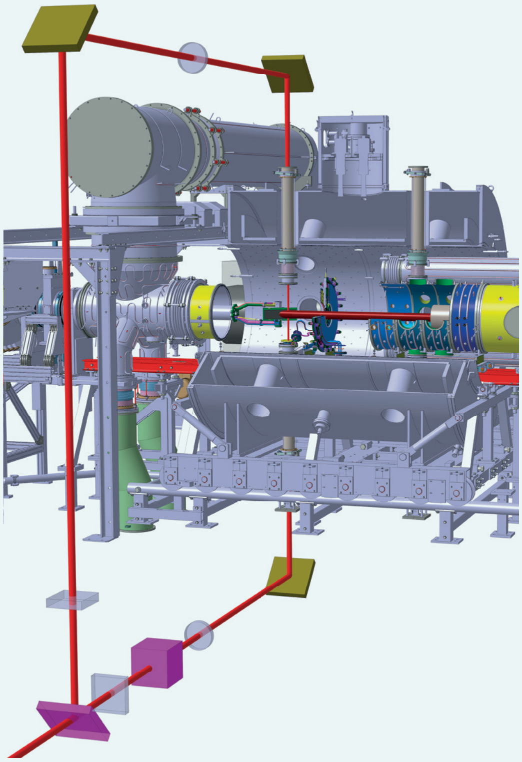


Figure 4.2. Collective Thomson Scattering system on Magnum-PSI with a multi-pass laser system. During the first roundtrip of the laser light the Pockels cell is activated, changing the light polarization and effectively traps the laser light in the ring cavity. To enable axial velocity measurements 2 half wave plates (grey) are installed to assure p-polarization in the plasma center. The laser beam will pass the scattering volume multiple times and increase the scattering energy with a factor of 15.

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[47] H.J. van der Meiden et al., Appl. Phys. Lett.**109**, 261102 (2016)

Other PSI-lab facilities

In addition to Magnum-PSI, a number of research setups and diagnostics in the PSI lab each focus on different aspects of plasma surface interactions, see Table 4.1. The Pilot-PSI setup is built on the same principle as its larger counterpart Magnum-PSI, albeit with a lower magnetic field up to 0.2 T using Helmholtz coils. The setup utilizes a wall-stabilized arc plasma source with a smaller diameter channel and lower current resulting in a lower plasma flux than in Magnum-PSI. Complementing the PSI cluster are the flexible nano-PSI experiment for plasma-modification of surfaces, and a dedicated source test facility envisaged to further develop our the high-performance plasma sources required.

While many diagnostics can monitor the plasma and surface evolution during exposure, identifying what is happening in the near-surface region down to a few micrometers below the surface is much more difficult. DIFFER will therefore upgrade the Pilot-PSI experiment (Upgraded Pilot-PSI (UPP)) with direct access of the Ion Beam Facility (see next section) to the target, taking proper precaution and design to minimize the effect of the magnetic field on the ion beam spectra. The prospect of the principal ion beam analysis techniques in combination to the existing (plasma) diagnostic at Pilot-PSI suite will give a unprecedented *in situ* and *operando* insight in the material behavior under relevant plasma loading conditions.

Sidebar 12: Access to the PSI facilities

To ensure a large scientific impact and footprint for the PSI-research team, and establish national and international collaborations with top research groups in the field, DIFFER actively searches collaboration with external users and its Magnum-PSI and other PSI labs. An important external partner is EUROfusion, which funds a set number of experimental days on Magnum-PSI and Pilot-PSI and allows the European PSI community to request urgent access on pressing issues in plasma surface interactions relevant for the ITER design team.

Researchers from EUROfusion and other partners can express their interest for experiments via the website or through direct contact with the Group Leaders of FFI and PMI. Although this mode of operation was satisfactory, we aim at establishing an international program committee for the evaluation of external proposals. Evaluation criteria are scientific and technical soundness, relevance for the EUROfusion Roadmap, and the motivation to use the unique PSI facilities at DIFFER.

https://www.differ.nl/research/fusion-facilities-and-instrumentation/magnum-psi#performing-research

4.2 Multi-disciplinary lab facilities for fundamental energy research

Fundamental research on the future challenges in converting and storing sustainable energy requires a multidisciplinary approach and expertise (see Chapter 3). In addition to the PSI facilities, DIFFER strives to make a dedicated, flexible lab-infrastructure of table-top sized set-ups available in order to elucidate processes and materials behavior. This dedicated infrastructure includes laboratories for research into chemistry, optics, materials and surfaces, and plasmas. In addition to these permanent labs, DIFFER has prepared several multi-purpose flex-labs to allow for the quick kick-off of promising exploratory projects.

Chemistry laboratories

The two chemistry labs are dedicated to the fabrication of (photo-)electro-catalytic and photo-electrochemical materials as well as nanoparticles with plasmonic properties. These labs have been equipped with fume hoods for wet chemical processing and preparation of catalysts, core-shell nanoparticles, electrodes and electrolytes of electrochemical cells. Several furnaces of different shapes and sizes are available to anneal and treat particularly ceramic materials.

One chemistry laboratory will enable researchers to characterize the (catalytic) behavior of new electrolytes and new materials under exposure to gases and/or light. For this purpose several transparent and darkened enclosures have been installed in which such electrochemical reactors or photo-catalytic devices can be developed and tested in operation, or studied while exposed to electrodeless plasmas to enhance the chemical activity.

The other laboratory is equipped with an integrated optics lab in addition to the chemical infrastructure. That unique combination of a chemistry and optics lab is essential to unravel and understand the plasmonic properties and behavior of nanoparticles under light exposure ranging from white light sources to femtosecond (fs) laser pulses.

Sidebar 13: Membrane reactor for plasma-aided electrochemical conversion

DIFFER is developing an all-electric single-reactor technology combining the strengths of electro-catalysis and plasma activation in the conversion of sustainable energy. The aim is to improve the reaction kinetics and/or the selectivity of uphill electrochemical reactions (such as fixation of N_2 or CO_2 by water), through plasma excitation of the molecules.

The figure below illustrates the case of a plasma aided electrochemical device for ammonia synthesis from water and nitrogen. The conventional electrochemical approach suffers from low selectivity for ammonia production vs the undesired hydrogen evolution reaction. It has been identified that the rate of this process needs to be improved by a factor of 50 in order to be commercially viable[48]*. The role of plasma in the DIFFER's approach is to activate nitrogen and shift the selectivity towards ammonia synthesis even at higher current densities and thus improve the overall production rate to commercially viable levels.*

Industrial ammonia synthesis catalysts (Fe, Ru) need to be efficient in both the dissociation of N_2 and the hydrogenation of N-atoms. In DIFFER's approach these two steps are separated and therefore (cheap) hydrogenation catalysts (e.g. Ni, Co based materials) will be explored as candidate materials. In addition, a proton conducting membrane operating at low (e.g. Nafion or PBI based polymeric electrolyte) or intermediate (e.g. BZY ceramic electrolyte) temperatures will be used for extending the operating temperature window.

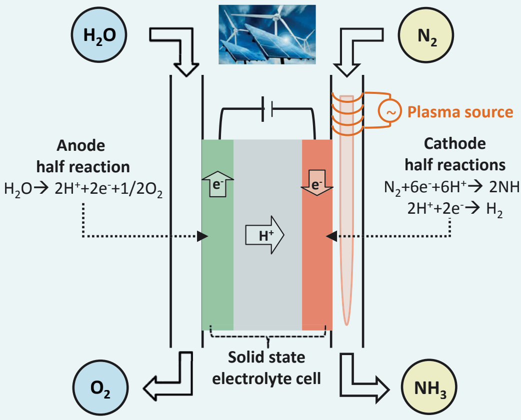

Figure 4.3. Plasma aided electrochemical setup for ammonia synthesis via water dissociation and N_2 fixation in a single all electric reactor. In the left hand side of the device, water is dissociated into O_2 and protons, The protons are transferred through a proton conducting membrane driven by an electrical potential (powered by renewable electricity). In the right hand side of the device, protons, electrons and N_2 react to produce ammonia.

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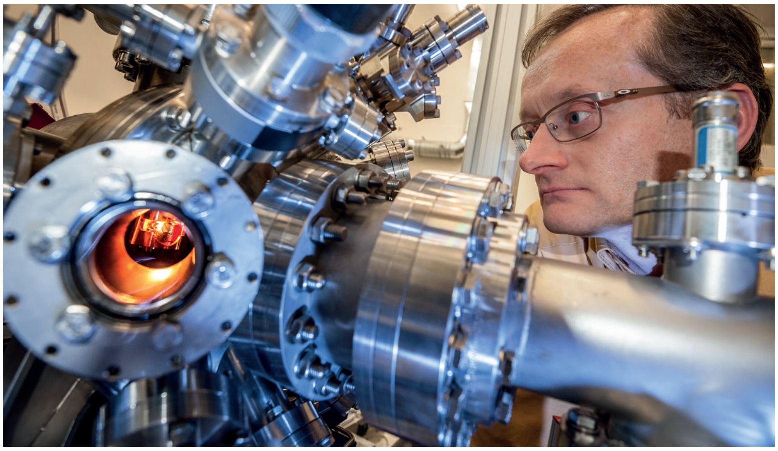
[48] A.R. Singh et al., ACS Catalysis **7**, 706 (2017)

Optics laboratory

The optics lab[49] will specifically accommodate all pulsed high-intense femtosecond laser equipment from visible to far-infrared range. Short laser pulses particularly allow for both the monitoring of processes with short lifetimes, such as charge carriers in materials, and for stimulating light-matter-interaction. The short (fs) laser pulses are detrimental for both selective excitation and monitoring the temporal behavior of molecular vibrations on material surfaces. Similarly, infrared and terahertz-radiation may lead to vibrationally excited surface species that also may enhance chemical reactions and selectivity.

Materials and surface laboratory

The Materials and Surface Science lab is built around dedicated *in situ* and *ex situ* materials analysis techniques. Several high and ultra-high vacuum systems for the deposition and treatment of materials are available. A dedicated plasma source producing well-defined and high fluxes of radicals and/or ions is available to expose catalytic materials to excited species while the interactions can be studied and characterized *in situ* and *operando*. These type of surface studies are typically carried out under very well-defined vacuum-conditions whereas industrial processes are operated at elevated pressures. The ambition is therefore in the future to study surface processes not only under vacuum conditions but also under ambient atmospheres. Moreover, we plan to further extend the in-house analysis techniques and develop them into nanomaterials characterization facilities, including electron microscopy, as well as extend the fabrication technologies with thin film deposition techniques for metals and oxides.



Plasma devices laboratory

DIFFER has extensive experience with plasma sources to generate (molecular) discharges across a wide range of pressures from a few Pascal up to atmospheric pressure, and in the frequency range from a few kHz up to GHz. These plasma reactors can be operated on various gas mixtures to study various plasma-assisted chemical conversion schemes. Also modification and functionalization of surfaces and materials by means of reactive plasma environments is studied for e.g. gas-separation purposes. These plasma reactors have optical access for active and passive laser spectroscopy to characterize molecular plasmas over the entire spectral range between 200 nm and 12000 nm. The “fingerprint” mid-infrared range (> 3000 nm) is of especially high importance for the analysis of molecules in the gas phase or adsorbed on (catalytic) surfaces. Moreover, the unique parameters of the tunable mid-infrared laser will make the selective vibrational excitation of molecules possible

The planned expansion of the plasma devices lab involves the upscaling of research-scale reactors into prototypes of 5-50 kW size and the application of mature semiconductor technology to enable pulsed modes of operation. Moreover, special attention will be given to the integration of catalytic and/or gas separation process steps, as an important step towards a working energy device.

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[49] At the moment of the writing of the Strategic Plan, the conditioning and temperature stabilization of the optics lab was still to be improved..

Access to external facilities

A complimentary and comprehensive suite of surface analysis and characterization tools is available at the NanoLab of the Eindhoven University of Technology (TU/e). This includes tools such as high-resolution SEM and optical microscopy, X-ray Photoelectron Spectrometry (XPS), X-ray diffractometer (XRD), surface profilometry and ellipsometry, and focused ion beam SEM (FIB-SEM). Specialized techniques such as scanning tunneling microscopy (STM) and transmission electron microscopy (TEM) are available in collaboration with partners within the TU/e.

4.3 Ion Beam Facility for dedicated material analysis

The Ion Beam Facility at DIFFER is built around a 3.5 MV singletron ion accelerator and is currently connected to various experimental setups (Figure 4.4). The available analysis techniques provide detailed insights into the processes on and below material surfaces. This information is crucial for the DIFFER research focusing on active energy system and devices, but the facility will also be available to accommodate researchers from other communities. For that aim, a stand-alone ion beam analysis station is available to external users for routine ion beam measurements with a variety of nuclear analysis techniques.

The connection to the target exchange and analysis chamber of Magnum-PSI enables an ion beam analysis capability to locally probe material composition and obtain elemental depth profiles for in vacuo studies, for instance to investigate fuel retention in nuclear fusion reactor walls.

DIFFER’s ambition is to enlarge the scope of the facility to *operando* measurements, to address research question in both Fusion Energy and Solar Fuels themes. By connecting the ion beam to Upgraded Pilot-PSI (station II in the figure), ion beam characterization of materials under extreme (plasma) environments will become available. This will prove relevant for research into a wide range of energy systems, from nuclear fusion to generic plasma catalysis to electro-catalysis.

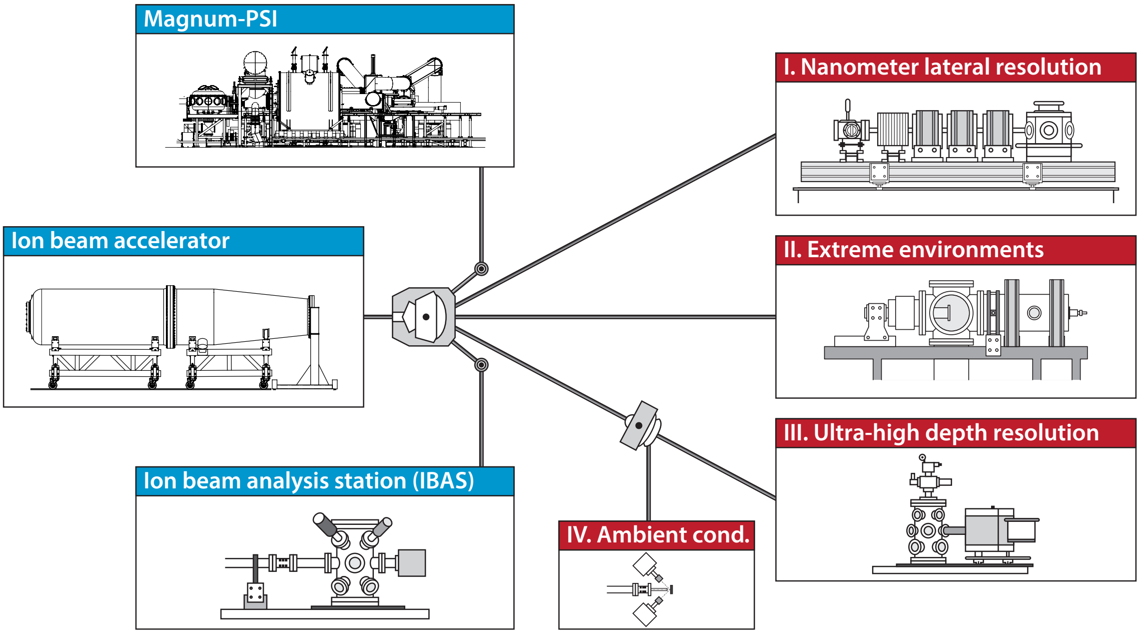


Figure 4.4. Schematic representation of the accelerator and the available beam lines (blue) and envisaged stations (red). Several ion beam analysis techniques, such as Rutherford Backscattering Spectroscopy (RBS), Elastic Recoil Detection (ERD), Nuclear Reaction Analysis (NRA), Particle Induced X-ray Emission (PIXE) and Particle Induced Gamma-ray Emission (PIGE), are available to investigate the composition of the exposed materials in a fully non-invasive way.

Adding to this, DIFFER will further develop new facilities capable of *in situ* and *operando* studies, in particular using the Ion Beam Facility complemented by other (optical) *in situ* and *operando* analysis techniques for the study of energy systems in general. A NWO Groot proposal will be prepared in close collaboration with DIFFER's research and industrial partners.

Plans for three additional *in situ* and *operando* end-stations are being developed to achieve state of art capabilities with respect to (sub-micron) lateral resolution (station I), ultimate depth resolution (station III), and ambient conditions (station IV). This allows for *operando* characterization of uptake and diffusion of mobile species in materials, and of evolution of lateral stoichiometry and inter-diffusion.

Sidebar 14: Ion beam analysis (IBA) on the Upgraded Pilot-PSI

In the Upgraded Pilot-PSI (UPP) we can obtain an understanding of tritium retention in the divertor wall by registering the uptake of deuterium in tungsten as a function of depth and time. In effect we aim to make a movie of the deuterium profile during extreme, relevant for the divertor of a nuclear fusion reactor, plasma loading conditions (~10^{23} m^{-2} s^{-1}). For that purpose, we have to realize in situ *and* operando *ion beam diagnostics, in particular Elastic Recoil Detection (ERD) and Nuclear Reaction Analysis (NRA).*

In the case of these operando *ion beam analysis measurements on UPP, there are a number of practical complications. The greatest challenge will be to maintain a good detector resolution, while the extremely sensitive particle detectors for IBA are subjected to severe amounts of electromagnetic fields, light and heat making the use of custom housings for the detectors necessary. In order to achieve fast measurements, a very large acceptance angle will be needed. Focusing of the incoming $^{3}He^{+}$ (NRA) or $^{4}He^{+}$ (ERD) ion beam into a well-defined spot on the target is a significant challenge. The ions, produced in DIFFER's singletron at a 25 m distance, will experience ionization and scattering due to their interaction with the abundant gas molecules and will have to be shielded from a strong and varying magnetic field originating from nearby Magnum-PSI as well as from UPP itself. Finally, the pathway of the particles that travel from target to detector will depend on both their energy and charge state. This will result in distorted energy spectra which will have to be reconstructed to obtain proper depth profiles by using spectra of reference samples.*

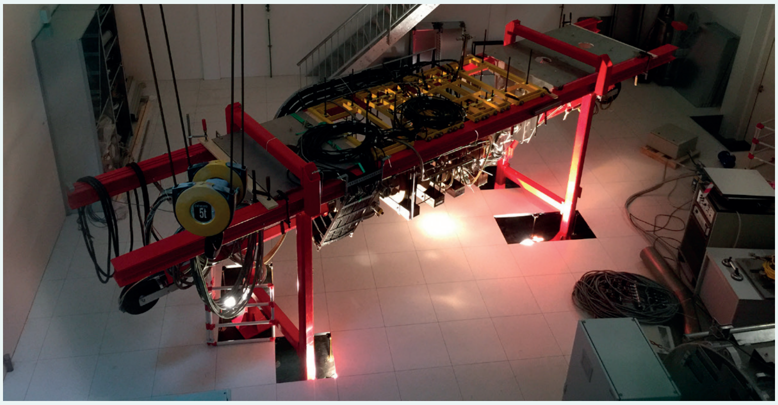


Figure 4.5. Upgraded Pilot-PSI experiment

4.4 Computational infrastructure

Use and co-development of codes

The computational and modeling groups at DIFFER use an array of codes to perform their research.

The Fusion Energy theme is a prominent user and co-developer of codes for the analysis of particle and energy transport in tokamaks. These include the nonlinear gyrokinetic turbulence code GENE, the quasilinear gyrokinetic transport model QuaLiKiz, and the integrated modeling suites for the plasma core CRONOS and JINTRAC. The latter have applications towards studies of detached plasmas in tokamaks.

To enable rapid scenario optimization and control applications, multi-layer perceptron neural networks are developed within the TensorFlow framework, with the goal to achieve an orders of magnitude acceleration of the RAPTOR control-oriented tokamak simulation suite and even allow real-time estimation of the turbulent fluxes.

In addition to (co-)development of codes, DIFFER is an active user of e.g. the 3D nonlinear MHD code JOREK for the study of plasma instabilities and their stabilization.

To stimulate wide adoption of in-house developed codes by the nuclear fusion community, DIFFER has realized implementation of the TORAY and RELAX for the modelling of electron cyclotron heating and current drive in the European Integrated Tokamak Modelling platform. This work was carried out within the EUROfusion work package code development (WPCD). Likewise, the institute pursues adoption of the in-house developed code EUNOMIA for the 3D Monte-Carlo modelling of neutral particles in the SOLPS-ITER package for studies of the scrape-off layer and plasma-surface interaction.

The Solar Fuels theme uses the VASP software to perform Density Function Theory (DFT) atomistic simulations of the electrochemical overpotential at metal oxide surfaces. Additional code is currently written in-house using MATLAB/SIMULINK,to calculate electrochemical data, such as electrochemical impedance data, current - voltage plots and surface species.

The Bari hybrid particle-in-cell with Monte Carlo collision/fluid model is used to simulatecapacitively coupled radio frequency plasmas in hydrogen. This model was developedand extended by group leader Dr. Paola Diomede, who is also co-developing a code to solve the Fokker-Planck equation for the vibrational kinetics of the asymmetric mode of CO_2 molecules.This code is part of a big project to model the chemistry of CO_2 and other molecular plasmas and will be included in a complex model currently under development.

To perform quick benchmarks and predictions for experiments at DIFFER, a model for the chemical kinetics of CO_2 plasmas has been developed using the ZDPlasKin software, extended to include the effect of gas flow and coupling with the input power density.

Access to computing facilities

A variety of computing facilities are used. Less demanding tasks are performed on the in-house computing cluster and the local clusters at TU/e. The next step up are the LISA and CARTESIUS clusters at SURFsara in Amsterdam. For High Performance Computing, DIFFER has access to European supercomputers such as the Edison, Cori and Marconi facilities, either through the PRACE partnership or through EUROfusion.

Sidebar 15: Machine Learning

Machine learning techniques are emerging as powerful tools for accurately capturing structure from data. With the advent of high-performance computing, advanced neural network topologies, training algorithms, and heuristics, machine learning methods are claiming a place in the standard research toolbox for prototypical applications such as regression and pattern recognition. Currently two projects are carried out, both aiming to accelerate computation beyond any conventional method presently in use, and facilitating breakthrough discoveries in their respective fields.

- *New deep learning neural networks will be developed trained on accurate and reliable large-scale quantum chemical data generated from density functional theory (DFT) calculations on materials for different target applications. The aim is to fine-tune our machine-learning model in an effort to quickly and accurately predict the key physical properties of new materials within a chemical domain, in particular for molecular photo-catalysts to convert* CO_2.
- *Feedforward multilayer perceptron neural networks will be applied to emulate tokamak turbulent transport models via regression of quasilinear gyro-kinetic transport model outputs. The neural network output then has the unprecedented promise to provide plasma turbulent transport coefficients in real-time, applicable within the RAPTOR tokamak simulator for discharge optimization and control.*

Key to both projects are the steps of initial data generation or sourcing; data pre-processing and filtering; and neural network training and validation. Existing libraries and neural network training workflows, developed by the substantial external machine learning community, will be applied. The challenge is in honing the skills and intuition necessary for application of the existing techniques for our specific applications.

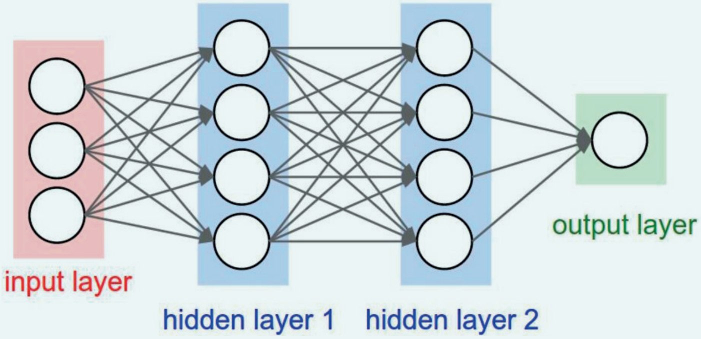


Figure 4.6. Standard neural network topology (reduced for simplicity), as applied for regression or pattern recognition. The hidden layer nodes correspond to bounded nonlinear functions (e.g. hyperbolic tangents), and the arrows (trained weight coefficients) correspond to linear sums. For our applications, the input layer typically corresponds to known or measured physical properties of the system in question, and the output layer to an a priori unknown attribute of the system.

5 ACTIVE ROLE IN DUTCH ENERGY COMMUNITY

Politics and society recognize the urgency to accelerate the energy transition - and meet the climate targets set at the COP conferences in Paris and Marrakech[8]. Bringing the various options in energy technology to economic feasibility throughout the transition requires continuous attention and scientific input. As the premier strategic instrument of NWO on energy research, it is upon DIFFER to connect the various national disciplines and actors in this field.

In doing so, DIFFER pursues the realization of:

- **joint activities** between fundamental and applied research institutes;
- **agenda setting** on energy research by connecting and contributing to the relevant platforms and networks;
- **continuous awareness** of the role of (basic) energy research in meeting the climate targets for the short-, mid- and long-term.

5.1 Joint activities

Since sharing knowledge is a best practice in scientific conduct DIFFER organizes a range of joint activities bringing together researchers with various backgrounds. These provide participants with a clear picture of the different approaches pursued, provide fertile soil for inspiration and insights, and spark future collaborations. These activities focus on connecting disciplines in use-inspired fundamental energy research and bring together all relevant actors in the innovation chain, from basic and applied researchers to developers at enterprises and industries.

To further seek and exploit the synergy in collaborative acceleration of energy technology development, to enable a timely societal energy transition, DIFFER pursues future joint activities based on its research portfolio, leading to:

- a **national long-running research program on Electrochemical Conversion and Materials**, in which technology innovation and industrial scale-up go hand in hand. This requires collaboration of partners from academia, applied research and industry to meet system targets for the mid- and long-term;
- a **national nuclear fusion program**, strengthening and positioning the Dutch research in international context, and providing opportunities to expand the dedicated expertise to other fields;
- a **clear positioning of *in situ* and *operando* studies** in the fields of energy research and beyond. Dedicated workshops are envisaged to investigate and tackle specific research questions in a joint approach of DIFFER and other relevant national laboratories;
- **intensification of collaboration with regional small and medium-sized enterprises** in the Eindhoven region and beyond, for example by expanding collaboration with polytechnic schools that are already cooperating with these companies.

DIFFER is very well positioned to succeed in these efforts thanks to its extensive network. The institute has established collaborative energy research networks with national and international academic partners and contributed to the preparation of new basic science programs on energy research. Use-inspired research and development programs and projects were realized with enterprises and industries. Furthermore, ties were strengthened with polytechnic schools, for instance through the shared appointment of a Fontys – DIFFER lector.

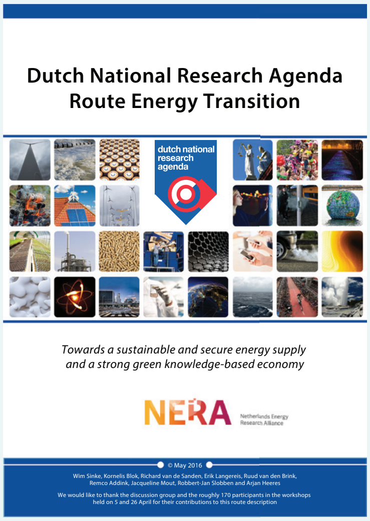
Sidebar 16: The Netherlands Energy Research Alliance

DIFFER is an active member of the Netherlands Energy Research Alliance (NERA[50]), the Dutch national consortium of universities and research and technology institutes with a considerable effort in energy research. DIFFER director Prof. Van de Sanden chairs the NERA scientific board and Dr. Langereis is active member of the NERA working group.

The strength of NERA is that it represents a large part of the innovation chain, from technology readiness levels 1 to 7 (of 9), which is crucial to facilitate and accelerate innovation. Via NERA, DIFFER is able to establish awareness on the role of fundamental energy research for the energy transition, prepares documents for agenda setting for energy research, and organizes workshops and other activities joining researchers of different disciplines.

Under the umbrella of NERA, DIFFER chaired the process to consult all stakeholders in the energy community and formulate the Energy Transition route of the Dutch National Research Agenda (NWA[51]). This describes the scientific needs and challenges regarding (the acceleration of) the transition towards a sustainable and secure energy supply and a strong green knowledge-based economy in 2050[52]. Supported by ten transition-related challenges, the message of the route is to take an integrated approach to technical, social, economic, legal and spatial planning aspects.

This cross-sectoral and multi-disciplinary approach is prone to materialize within NWO and the Topsectors roadmaps. Moreover, via NERA it will be brought to the European context of the European Energy Research Alliance (EERA[53]) which provide input to the EU Strategic Energy Technology Plan (SET-plan[54]) and research program H2020, as well as international initiatives like Mission Innovation[55].



Dutch National Research Agenda
Route Energy Transition

Towards a sustainable and secure energy supply
and a strong green knowledge-based economy

© May 2016

Wim Sinke, Kornelis Blok, Richard van de Sanden, Erik Langereis, Ruud van den Brink,
Remco Addink, Jacqueline Mout, Robbert-Jan Slobben and Arjan Heeres

We would like to thank the discussion group and the roughly 170 participants in the workshops held on 5 and 26 April for their contributions to this route description

Figure 5.1. The Energy Transition Route in the Dutch National Research Agenda.

5.2 Agenda setting

To create opportunities for research funding on the interdisciplinary theme of sustainable energy, it is crucial to provide concise input to agenda setting initiatives from a basic research perspective, both nationally and internationally. To this end DIFFER has become a representative voice for fundamental energy research, in good agreement with other players in the innovation chain. DIFFER will further develop its pro-active role in relevant initiatives, platforms and networks.

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[50] www.nera.nl
[51] www.wetenschapsagenda.nl
[52] https://www.nera.nl/ten-challenges-for-the-energy-transition
[53] www.eera-set.eu
[54] https://ec.europa.eu/energy/en/topics/technology-and-innovation/strategic-energy-technology-plan
[55] http://mission-innovation.net/

DIFFER supports the approach to put emphasis on the *energy functionality* needed in a future sustainable energy system, rather than on the *technology* providing it. This implies the focus will have to be on light & equipment, low- and high-temperature heat, and transport & mobility[56]. Especially for long-term agenda setting (> 15-20 years), it is vital to create a fair playground for incrementally improving existing technologies as well as for novel innovative technology routes that currently are at relative infancy. In a national context DIFFER will do so through:

- an **active and recognized role in all NWO sustainable energy research initiatives**, so also those beyond the scope of DIFFER's own research portfolio. This is in line with the necessity of an integral approach of technical, social, economic, legal and environmental challenges as was put forward in the Energy Transition route of the Dutch National Research Agenda;

- strongly **advocating the role of fundamental energy research** as an important enabler of energy innovation in the mid to long term. DIFFER will therefore strengthen the ties[57] with the Ministry of Economic Affairs and its Topsectors Energy, Chemistry and High-Tech Systems & Materials, and further develop its role in the Netherlands Energy Research Alliance (NERA).

In the field of energy conversion and storage a range of viable technology options has to be considered in the light of specific (niche) requirements. As a consequence, DIFFER positions its Solar Fuels research on converting energy to chemical bonds as part of a systems approach, rather than as an individual technology. Successful examples of this systems approach will be used to draw attention to the relevance of fundamental research as an enabler for the acceleration of technology innovation for energy storage and conversion. In short DIFFER aims to:

- **incorporate a long term perspective on possible technology scenarios for storage and conversion** by influencing research agendas nationally and internationally;

- be **an active member of platforms on energy conversion**, such as the Dutch regional platform Brainport, and by providing input to the European Energy Research Alliance (EERA) to affect the European Sustainable Energy Technology (SET) plan and the Horizon2020 (and beyond) research programming.

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[56] Report Rijk zonder CO_2: *naar een duurzame energievoorziening in 2050* of the "Dutch Council for the Environment and Infrastructure" (RLI - Raad voor de leefomgeving en infrastructuur, http://www.rli.nl/publicaties/2015/advies/rijk-zonder-CO_2-naar-een-duurzame-energievoorziening-in-2050

[57] By taking a leading role in the Energy agenda setting. For example, Prof. Richard van de Sanden is currently the chair of the NERA Scientific Board and the chair of the advisory committee on Electrochemical Conversion & Materials.

In a similar way, the role of nuclear fusion energy needs to be positioned in terms of the system need for large(r) scale electricity and high-temperature heat production in a sustainable energy society. To date the global concerted effort in the field of fusion energy is focused on the development of ITER and its successor DEMO, as the most promising concepts for large scale commercial nuclear fusion energy generation. However, several other approaches might deserve attention, such as the stellarator concept and specific elements in support of small-scale nuclear fusion reactors. DIFFER strives to:

- continue in its role as **the Dutch beneficiary in the EUROfusion consortium** in coordinating the Dutch nuclear fusion research community and its efforts
- provide direct input to **EURATOM** and the European research agenda Horizon 2020
- support the development of new approaches to nuclear fusion reactors, such as the high magnetic field tokamak from MIT.

Sidebar 17: EUROfusion

The European nuclear fusion research effort is committed to the ITER and DEMO projects. In 2014 the agreement on the EUROfusion consortium was signed by 26 European Union member states, plus Switzerland. EUROfusion adopted the `Roadmap to the realization of nuclear fusion energy' which outlines the steps necessary to produce electricity from nuclear fusion by 2050. It identifies ITER and DEMO as key facilities for reaching this goal and concludes that "a reliable solution to the problem of heat exhaust is probably the main challenge towards the realization of magnetic confinement nuclear fusion".

DIFFER is the single Dutch beneficiary in EUROfusion and acts as the linking pin for Dutch knowledge institutes to participate in the EUROfusion program. At present CWI, Eindhoven University, University Twente and NRG are linked third parties while new linked third parties are foreseen to participate. On request of the EUROfusion general assembly, the Eindhoven based European mobility and education program for MSc students in nuclear fusion "FUSENET" will become a linked third party, and negotiations with the Delft University of Technology are underway.

EUROfusion uses the DIFFER Magnum-PSI facilities for its materials program (typically 500 experiments per annum). It is foreseen that this effort will be continued in the coming years. DIFFER scientists participate in experiments and analysis in the Joint European Torus (JET) and the medium sized tokamaks ASDEX Upgrade, TCV and WEST. For 2017-2018 experiments are also foreseen in the Wendelstein 7X stellarator in Greifswald that has just commenced operation.

5.3 Awareness

DIFFER promotes widespread awareness of the essential role for fundamental research in realizing the energy transition. To ensure lasting support for this message, the institute will strengthen its ongoing dialogue with stakeholders including policy makers, funding agencies, energy professionals, fellow scientists, future researchers, and the public in general.

Working with its partners and within established networks, the institute aims to become the prominent voice for fundamental energy research in the Netherlands on the basis of its recognized scientific expertise and that of its researchers. DIFFER will:

- seek opportunities to **host, organize and participate in public events** related to sustainable energy, to represent fundamental energy research for a wide audience;
- **increase the institute's public visibility** by actively engaging with journalists and generating media exposure, and positioning its members as experts in the public debate via e.g. op-ed pieces or social media presence;
- use successful examples of **joint research activities as showcases** to demonstrate the added value of applying fundamental insights to realize breakthrough energy technologies;
- seek closer **collaboration with student project teams at universities or polytechnic** schools to develop appealing examples of innovative sustainable energy technology.

6 INSTITUTIONAL MATTERS

To realize its strategic goals in energy research, DIFFER operates a skilled in-house Support Facilities division. This chapter describes DIFFER's administrative and general support groups, including the HRM department, project office, management support and communication group; and the institute's technical support groups. Finally, this chapter presents a financial outlook for the institute.

6.1 Administrative and general support

a. Human Resource Management

The institute's strategy for Human Resource Management is based on DIFFER's mission and strategic goals, and focuses on:

- enabling scientific excellence in a multidisciplinary environment;
- stimulating collaboration, both internal and external;
- maintaining a viable, healthy organization with a diverse, highly educated, well trained staff and a sound financial strategy.

DIFFER aims for a professional, responsible and motivated workforce. To achieve this the institute maintains an open, positive and creative environment where participation is encouraged and stimulated at every level of the organization.

Organization and leadership

The DIFFER organization is designed to make science flourish. Support facilities are organized mean and lean, and cost-effective. Characteristic to DIFFER's governance is the flat organization structure. Group leaders and heads of departments play a key role in the execution of DIFFER's policy, particular in supporting, mentoring, coaching and informing employees. A tenure track program is in place to develop early career talent to the level of group leader in the course of five years. Tenure trackers are actively mentored by senior group leaders and theme leaders in regular bilateral discussions. Furthermore, the tenure trackers and group leaders present their research program and progress during the annual Grand Staff meeting.

DIFFER maintains a sound ratio of 60% permanent and 40% temporary staff, in accordance with its funding structure. This enables DIFFER to be agile and bring in new knowledge and skills on a regular basis.

Employability and development

Both in the interest of individual employees and DIFFER as a whole, the institute strives to enhance the employability of its employees. Courses to enhance knowledge and skills are available to all personnel, including a special package for PhD students (facilitated through NWO). To facilitate collaboration and knowledge exchange with former employees, trainees and guests, an alumni program will be established.

Recruitment

Strategic personnel planning is in the interest of DIFFER, to structurally embed valuable knowledge and skills within the groups. This involves e.g. targeted recruitment of specialists in key areas of DIFFER's multidisciplinary program, such as physics, chemistry, engineering and materials science.

Diversity

DIFFER strives to achieve a diverse workforce to develop talent and creativity by bringing together different perspectives in a respectful workplace. An employee survey held in 2016 indicated that increasing cooperation and solidarity is a key instrument to strengthening the institute. As a result of this, we will extend the introduction program and organize more informal meetings.

DIFFER also strives to maintain the well-balanced age structure in the institute, which is in good accordance with the age distribution of the working population in the Netherlands. DIFFER will define policy to safeguard knowledge and expertise of its work force, for example to structurally embed the expert knowledge developed by the PhD students.

Action will be taken to further diversify the institute's workforce, both by international recruiting and by pursuing a balanced gender ratio in the staff. DIFFER will carry out honest and transparent recruiting and selection procedures for her positions and, in cases of equal qualifications, will favor an increase in the diversity of its workforce. Staff members will undertake a diversity awareness training and selection committees for new employees will have at least one member trained in diversity awareness issues. As an example, in the case for gender diversity, the institute aims at a minimum of 20 percent representation of women in top positions (pay band 12 and higher) by 2020, as laid out in the NWO "20 in 2020" policy on gender balance.

b. Project office and management support

The management of DIFFER is carried out in a context of increasing complexity and growing demands on administration. As a consequence, the team supporting the management has recently been expanded to handle and safeguard all contracts. The rules of the European Union with respect to tendering in the procurement of equipment or services have to be followed in a growing number of cases. These procedures are expensive and time-consuming. The legislation with respect to safety of equipment and personnel and the protection of the environment is becoming more stringent and does have a considerable impact on the operation of the institute. All these developments require a further(modest) increase of the staff for management, management support, administration and maintenance support.

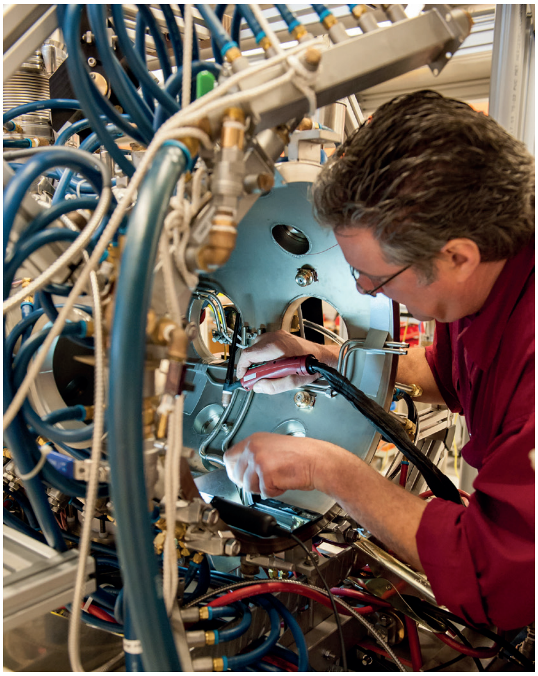
c. Outreach and communication

The DIFFER communications group aids the institute and its staff in creating and maintaining relationships with stakeholders. The aim of the group is to further increase DIFFER's visibility and recognition as a top class research institute and as the point of contact for everyone interested in fundamental energy research in the Netherlands.

In the communication efforts, emphasis is put on direct interactions with DIFFER's partners and on further boosting interactions within the institute. Recognizing that every employee of DIFFER is a possible communicator with stakeholders within and without the institute, the communications group aims to enable DIFFER employees in their role as ambassadors of the institute.

6.2 Technical support

DIFFER's technical support consists of highly experienced in-house groups for the design and manufacturing of experimental equipment, for electronics and software engineering, and for computer infrastructure support. The institute will maintain these groups at their present capacity and capabilities to assure continued high quality support for the research.



DIFFER is especially strong in the design and construction of state-of-the-art experimental set-ups, of which Magnum-PSI is the most striking example. Due to the multidisciplinary nature of the energy research at DIFFER, furtherreorientation within the technical support is envisaged to include disciplines such as chemical synthesis and material processing and characterization.

The Mechanical Techniques department of DIFFER consists of the sub departments Design Office and Mechanical Workshop. In close collaboration with the scientific staff and its research technicians, the design office designs and manufactures research and diagnostic equipment needed for scientific research. The group engineers use the software packages Catia V5 for the high-end 3D design and Simulia to simulate strength, stress, heat load and frequency behavior of mechanical structures.

In the mechanical workshop, manufacturing of designed equipment is done with several machines, including CNC milling and -lathing machines and a newly acquired wire-EDM machine. CAM software used as interface between design software and CNC machines is Hypermill. The group also has the knowledge and equipment required for vacuum and high temperature brazing and TIG and laser welding.

The DIFFER Electronics & ICT department consists of the subgroups Electronics, Software Engineering and IT-Support. The group provides electrical engineering, support and maintenance for the institute’s experimental setups, including the design of printed circuit boards with FPGAs and embedded microcontrollers, and development of power electronics in the domain from radio frequencies to GHz. Power electronics engineers are also involved in the operation of the new Ion Beam Facility. In addition the software engineers of the group develop control and data acquisition software for all experiments (CODAC) and software and data storage systems for the DIFFER experimental setups. Finally, the group supports and operates the DIFFER computer network, including workstations, servers, printers, software licenses, etc.

7 FINANCIAL OUTLOOK

In the following sections, the funding of the strategic actions presented in section 2.3 will be discussed.

Sidebar 18: Funding structure of the institute

The institute receives funding from three sources: the mission budget, research grants and contract research.

The mission budget *is the 'base' funding of the institute, granted by the NWO-I Board. The mission budget of DIFFER is comparable to universities' budgets for the basic operation for research efforts, such as buildings, permanent staff, basic support and overhead. The mission budget of DIFFER amounts to 8.446 k€ in 2018. In the mission budget, reservations are made to execute the strategy (500 k€/year). In addition, to stimulate collaboration with industry, matching money can be provided of up to 500 k€/year.*

Research grants *and Institutional programs and Industrial Partnership Programs (IPPs) support the temporary scientific staff (PhD students and postdocs), the temporary technical staff as well as running costs for equipment. It is a relatively stable source of income, depending on the approval of programs. Upon approval of a (new) program, its budget is guaranteed for the total running time of typically five years. For large investments, researchers can apply for additional NWO grants (the so-called NWO Groot call).*

Contract research *consists of all European funding (Euratom / EUROfusion / ERC) as well as industry related funding and funding from agencies such as TTW, RVO, M2I and NWO-personal grants such as VENI, VIDI and VICI.*

Action 1: Strengthening and further developing research in a programmatic and integral approach

DIFFER will finance the development of its Solar Fuels and Fusion Energy themes and its new explorative research from the Mission Budget (i.e. manpower and materials budgets). For extra impulses to the research (e.g. investments or extra manpower), the DIFFER staff will actively seek for research grants and/or contract research. The staff has shown to be effective in acquiring these funds over the last years.

The development of DIFFER's cross-cutting research approach will require extra resources for DIFFER to be successful and effective in the longer run. We estimate that this will require about 1000 k€ per year, which will be split between the two research themes (i.e. 500 k€ per year each). These additional and preferably structural resources will enable DIFFER to start national long-term collaboration in the form of two national programs coordinated by the institute on each of its research themes. National partners (i.e. universities and companies) will be attracted for additional funds and resources. The additional funding will cover PhD students, postdocs, technicians and material costs.

Setting up the new research group on control engineering will require additional and preferably structural funding, as no room is available in the current mission budget. An investment of 1000 k€ as a starter packet for a tenure tracker is foreseen. Further structural means of 120 k€ per year are required, consisting of personnel costs and material budget.

Action 2: Maintaining and further developing the world-class infrastructure

In further developing the Upgraded Pilot-PSI experiment and its Ion Beam Facility, DIFFER will apply for 'NWO Groot' investment funds to cover the costs of the necessary hardware and machine upgrades. The investment required will be about 4000 k€. Defining the details of the investment and preparation for the application is in progress.

Action 3: Connecting networks of scientific, educational, industrial and societal partners

Networking funds are made available through the mission budget of DIFFER and are estimated at 50 k€ per year.

Action 4: Coordination of energy research in the Netherlands

Funds for coordination activities will be made available through the mission budget of DIFFER, as is already the case for our Research Development Officer. The extra costs for the coordination activities are estimated around 50 k€ per year. This extra investment is mainly for hiring support for the organization of workshops and writing opinion essays or research proposals.

Action 5: Ensuring a viable, healthy organization

Funds for the training of our employees will be made available through the mission budget of DIFFER and are estimated at 50 k€ per year.

Summary

Most resources required for the period 2017–2022 can be covered by a combination of the mission budget, research grants and contract research. The important strategic actions to setup nationally coordinating research programs on Fusion Energy research (500 k€ per year) and Solar Fuels research (500 k€ per year), and a new control engineering group (120 k€ per year) can however not be implemented by the current mission budget, research grants or contract research. In the coming period, DIFFER will actively seek for additional and preferably structural resources to implement these strategic actions.

Concluding, DIFFER is in an excellent position to fullfil the majority of its strategic actions. However, if the required resources can be allocated, it will kick-start the implementation of the new strategy and greatly contribute to the success of DIFFER and the energy research in the Netherlands.

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