



DIFFER



ANNUAL REPORT 2018

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

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Plasma in Upgraded Pilot-PSI by UPP team

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PREFACE



Management team and head of HR



Left to right: Henk Tamsma (head of HR) and MT members Wim Koppers, Marco de Baar and Richard van de Sanden

It is a great pleasure to present the annual report 2018 of DIFFER, the Dutch Institute for Fundamental Energy Research.

When I look back on this past year, I am proud of the progress in our two research themes, Fusion Energy and Solar Fuels. Our research groups are operating at the top of their field with well-equipped laboratories and computational facilities. Interactions with the wider community are well established, whether with the experimental and computational experts from our national partners, in international collaborations to produce clean kerosene, or to harness the plasma in future fusion power plants. Notably, DIFFER's main experimental facility Magnum-PSI attracts attention from research groups around the world as it set a world record in plasma surface interaction studies.

The institute's credentials as national research institute allow us to take point in organising the essential networks for fundamental energy research in the Netherlands, such as the Energy Transition Route in the Dutch National Research Agenda NWA. Our researchers connect Dutch knowledge institutes to the European Horizon2020 programme EUROfusion, collaborate in the national energy research alliance NERA and advise the public-private Topsectors on promising directions to sustainable energy technology.

DIFFER's important national role was confirmed by the recent Portfolio Analysis of the collection of Dutch research institutes. As the national coordinator of fusion energy related research and with a similar position foreseen for our solar fuels programme following recommendations from the Portfolio committee and the recent Institute Evaluation, the future is bright for DIFFER.

The many highlights and interviews with ambitious researchers in this report speak for themselves. I wish you pleasant reading.

*Richard van de Sanden, director
Eindhoven, March 2019*

"I am proud of the progress in our two research themes, Fusion Energy and Solar Fuels."

ABOUT DIFFER

DIFFER is the Dutch Institute for Fundamental Energy Research, with the mission 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.

SCIENCE FOR FUTURE ENERGY

Humanity has an ever growing need for energy. Our current fossil-dominated infrastructure is not the optimal way to provide that need, since it depletes fossil resources and leads to climate change due to greenhouse gas emissions. Scientific research plays a key role in developing fully sustainable alternatives. As the national institute for fundamental energy research, DIFFER connects knowledge partners and industry to accelerate the transition to a sustainable society. Our research efforts focus on harnessing the energy of the sun in two ways: we look into Solar Fuels to store and transport solar energy directly, and try to mimic the sun itself by working on Fusion Energy as a clean, safe and inexhaustible power source.

Fusion Energy has the potential to provide concentrated, safe and clean energy from the process which powers the sun and stars. Our fusion research program addresses high priority topics described in the European Fusion Roadmap. This roadmap is established by the European Horizon2020 EUROfusion consortium to support the development of ITER, an international nuclear fusion reactor that aims to demonstrate the technical feasibility of using fusion as an energy source on earth. With our unique high flux plasma generator Magnum-PSI, we explore how the extremely hot fusion fuel interacts with the reactor wall. We also develop tools to understand and control the highly nonlinear plasma dynamics in ITER and its successors. Ultimately, our research is aimed at developing robust solutions that ensure the optimal performance of an energy plant powered by nuclear fusion.

Our program on **Solar Fuels** addresses the global challenge of storing and transporting energy in an efficient way by converting sustainable energy into chemical bonds. DIFFER investigates both the indirect conversion of sustainable electricity into hydrocarbon fuels, and a direct approach to convert solar energy into chemical bonds, using so-called photo-electrochemical cells as artificial leaves. DIFFER's cross-disciplinary research addresses both the synthesis and design of novel materials and of processes to obtain scalable, efficient and cost-effective systems. The resulting insights can also be applied to the broader topic of electrification of energy intensive processes in (chemical) industries, which currently rely heavily on fossil feedstock.

MAGNUM-PSI SETS WORLD RECORD PLASMA EXPOSURE

On Wednesday 21 March 2018, DIFFER's research facility Magnum-PSI set a new world record for the longest exposure of a material to the harsh plasma conditions in future fusion reactors. The facility exposed tungsten wall components to the equivalent of a full year of high power fusion operations in ITER, fifty times more than the previous record.

Even before the ITER fusion project starts full power operations, the 'staged approach' will already expose the reactor's tungsten divertor or exhaust system, to years of conditions comparable to those in a welding flame, on a space craft's re-entry heat shield, or at the surface of the sun.

How will ITER's exhaust system perform after such treatment? To find out, the ITER Organization and the European fusion research consortium EUROfusion proposed a "lifetime" experiment. Their facility of choice was DIFFER's Magnum-PSI, the only laboratory facility in the world that can reach the harsh plasma conditions expected in ITER's divertor and maintain them for a long time thanks to its superconducting magnet.

ITER provided a small mock-up of its divertor, which was exposed in Magnum-PSI during the summer of 2018. In just 19 hours of plasma exposure, the divertor mock-up received the same total fluence of 10^{30} particles per square meter as ITER will produce in a full year of experimental runs. During the exposure, the surface temperature was kept around 1200 °C and faced a high steady-state flux of roughly 1.5×10^{25} deuterium ions $m^{-2}s^{-2}$ and an average power load over 10 MW / m^2 .

The plasma exposure record shows Magnum-PSI's unique capability to investigate how the ITER wall material will evolve under plasma exposure. This is crucial to gauge future performance while the actual fusion reactor is being built.

Happy building award 2017

On 18 April 2018, DIFFER was awarded the Happy Building Award during the Building Holland event in the RAI exhibition centre in Amsterdam. This award celebrates the best new and sustainable buildings in the Netherlands. According to both visitors and employees, the new DIFFER building is a pleasant environment where people are happy to work and meet each other.

Institute manager Wim Koppers (second left) receives the Happy Building Award



PEOPLE HIGHLIGHTS



Marco de Baar

Marco de Baar heads ITPA working group

The International Tokamak Physics Activity (ITPA) has appointed DIFFER theme leader **Marco de Baar** as chair of its Realtime Specialists Working Group (RT-SWG). The ITPA is an international framework organised by the global ITER fusion project to coordinate fusion research. ITPA activities prepare the broad physics basis needed for ITER design and operation. DIFFER is honored by the appointment, as members of the ITPA groups are chosen by each ITER party as representative top experts of their sub-fields.



Mihalis Tsampas

Producing hydrogen from ambient humidity

Existing water splitting systems to produce hydrogen use liquid, purified water. **Mihalis Tsampas** in cooperation with Toyota Motor Europe was awarded an NWO LIFT grant to investigate a design for hydrogen production that uses sunlight and water from the ambient air. This would be ideal for remote areas or along roads without running water.

PhD theses 2018

Seven PhD candidates at DIFFER successfully defended their research thesis at Eindhoven University of Technology in 2018. Three theses were published by candidates from the Fusion Energy theme, and four by Solar Fuels candidates.

Professorships at TU/e

Two DIFFER researchers were appointed full professor at Eindhoven University of Technology (TU/e) in 2018.

Head of the Nonequilibrium Fuel Conversion group **Gerard van Rooij** received a professorship in sustainable plasma chemistry.

Director **Vianney Koelman** of the joint DIFFER-TU/e Center for Computational Energy Research (CCER) was appointed professor in the field of Computational Energy Research.



Vianney Koelman and Gerard van Rooij



Jonathan Citrin

EUROfusion grants

DIFFER tenure tracker **Jonathan Citrin** won one of 26 EUROfusion Enabling Research Grants for his group on Integrated Modelling and Transport. This project will investigate fast neural networks that can predict turbulent transport phenomena in fusion reactors.



Clockwise from top left:
PhD theses of 2018 by Damien Aussems, Dirk van den Bekerom, Stein van Eden, Fiona Elam, Anna Meshkova, Yaoge Liu and Vladimir Kvon.

Physicist **Isabel Krebs** was one of ten researchers to be awarded a prestigious EUROfusion Researcher Grant in 2018. She will join DIFFER to focus on understanding magnetic flux pumping, an effect that may offer the possibility of longer, more stable plasma discharges in future fusion reactors.



Isabel Krebs

RESEARCH

THEME FUSION ENERGY

Theme leader:

Marco de Baar

Research groups: 6

Science staff:

permanent staff 9
post-docs 9
PhD students 19
research engineers 13

Peer reviewed publications 55
Open access publications 44
PhD theses 3
Invited talks 42

Grants and prizes:

- EUROfusion Enabling Research Grant - Jonathan Citrin
- EUROfusion Researcher Grant - Isabel Krebs
- Plasma Sources Science and Technology highlight article - Paola Diomede
- Best TU/e Applied Physics MSc thesis - Oliver Linder
- NumFOCUS award for open source contribution - Karel van de Plassche
- AAPPs poster prize - Michele Marin

Industrial collaborations:

NL ASML, HIT
EU Research Instruments



DIFFER's Fusion Energy research directly addresses the challenges posed in the Energy Transition route of the Dutch Science Agenda (NWA).



Nuclear fusion, the process that generates heat inside the sun, has great potential as a concentrated, safe and clean energy source on earth. To achieve fusion on earth, we need to control the hot, turbulent fuel of charged particles (plasma) in a fusion reactor. Fusion Energy research at DIFFER is aimed at developing the advanced models and controllers to do this, and at finding out how wall materials for fusion reactors will interact with the extreme plasma conditions at the reactor exhaust.

DIFFER is strongly involved in the international fusion project ITER, which aims to demonstrate the technical feasibility of fusion energy. ITER is the first ever experiment where the power generated by the fusion reaction will exceed the power needed to maintain the reaction. DIFFER develops techniques to sense, predict and control the many possible instabilities in the hot, magnetized plasma in order to optimize the reactor performance.

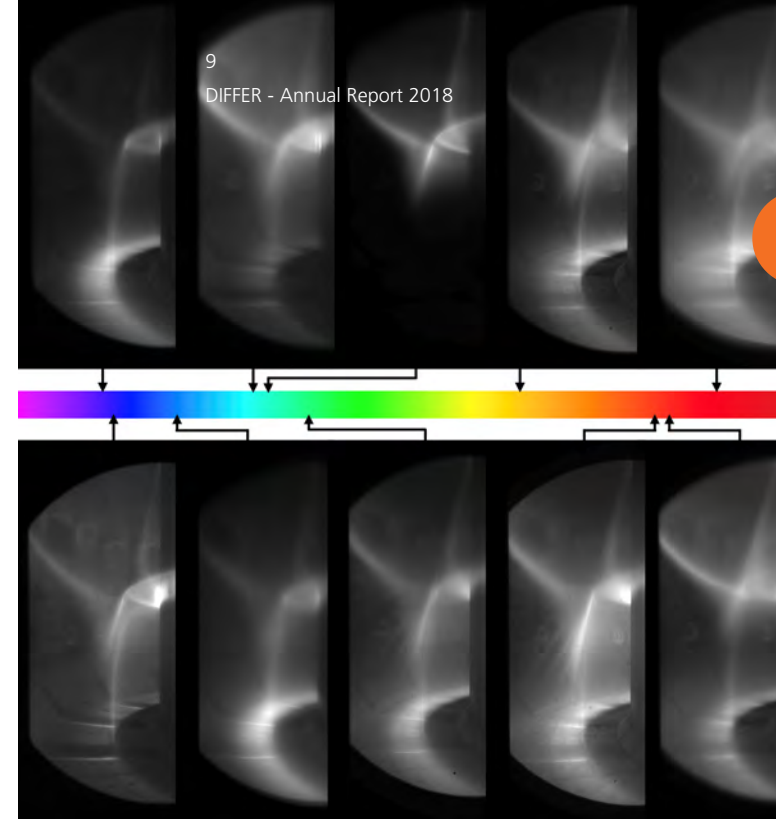
At the ITER exhaust, wall materials face extreme conditions in an environment similar to the surface of the sun or a spacecraft's re-entry heat shield. DIFFER's linear plasma device Magnum-PSI is the only laboratory facility in the world capable of exposing materials to such extreme plasma surface interactions. Our researchers study the effect of wall materials and develop new concepts for reactor components.



European connection

EUROfusion is the Horizon2020 research program on fusion research, with 30 consortium partners in the EU. As the Dutch point of contact in this program, DIFFER is the linking pin between Dutch researchers and companies and the international fusion community.

The research at DIFFER addresses two high priority topics in the European Fusion Roadmap, namely the mission plasma regimes of operation and the mission heat-exhaust systems. EUROfusion annually awards grants to excellent researchers in its field and DIFFER manages to regularly score these research positions.



MANTIS takes multiple images at different wavelengths through the same lens, allowing it to simultaneously monitor different processes at the plasma edge

To understand detachment, the MANTIS multispectral imaging system employs interference filters to divide visible light into very precise bands. Ten of those bands can be observed simultaneously to separate the light originating from different plasma processes. MANTIS also has real-time capabilities to analyze and combine its data streams to look for the locations where the dominant detachment processes occur. Those locations can be used in the reactor control systems to maintain the balance between fusion and exhaust power.

A testbed for models of transport in the plasma edge

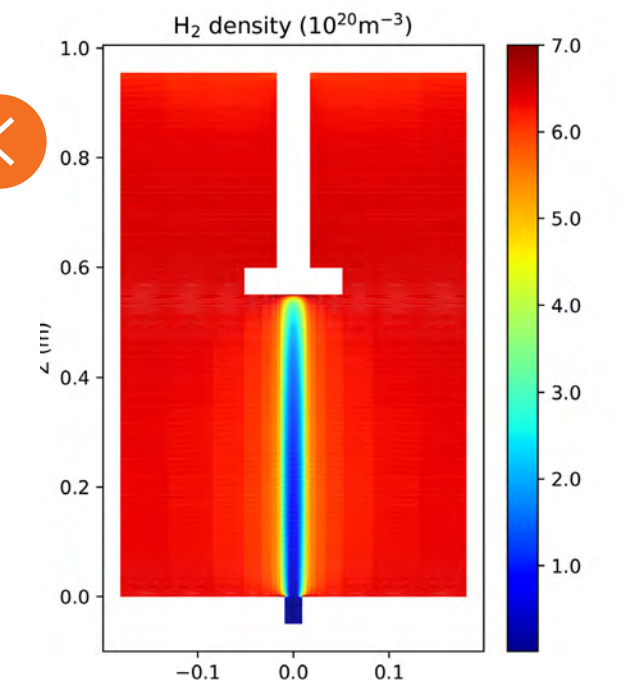
Linear plasma devices make excellent testbeds for computer codes that model transport phenomena in the plasma edge, because of their well diagnosed plasma parameters and simple geometry. In this work DIFFER researchers compared hydrogen plasmas in Pilot-PSI to the fluid/Monte-Carlo code Soledge2D-Eirene. Inside the plasma beam, the density of hydrogen molecules is lowered due to both elastic collisions with ions and dissociation by electrons. We were able to demonstrate that molecular dissociation is playing a bigger role in cooling edge plasmas than is usually assumed in simple models.

Studying divertor relevant plasmas in the Pilot-PSI linear plasma device: experiments versus modelling, Plasma Physics and Controlled Fusion 60, 12 (2018)

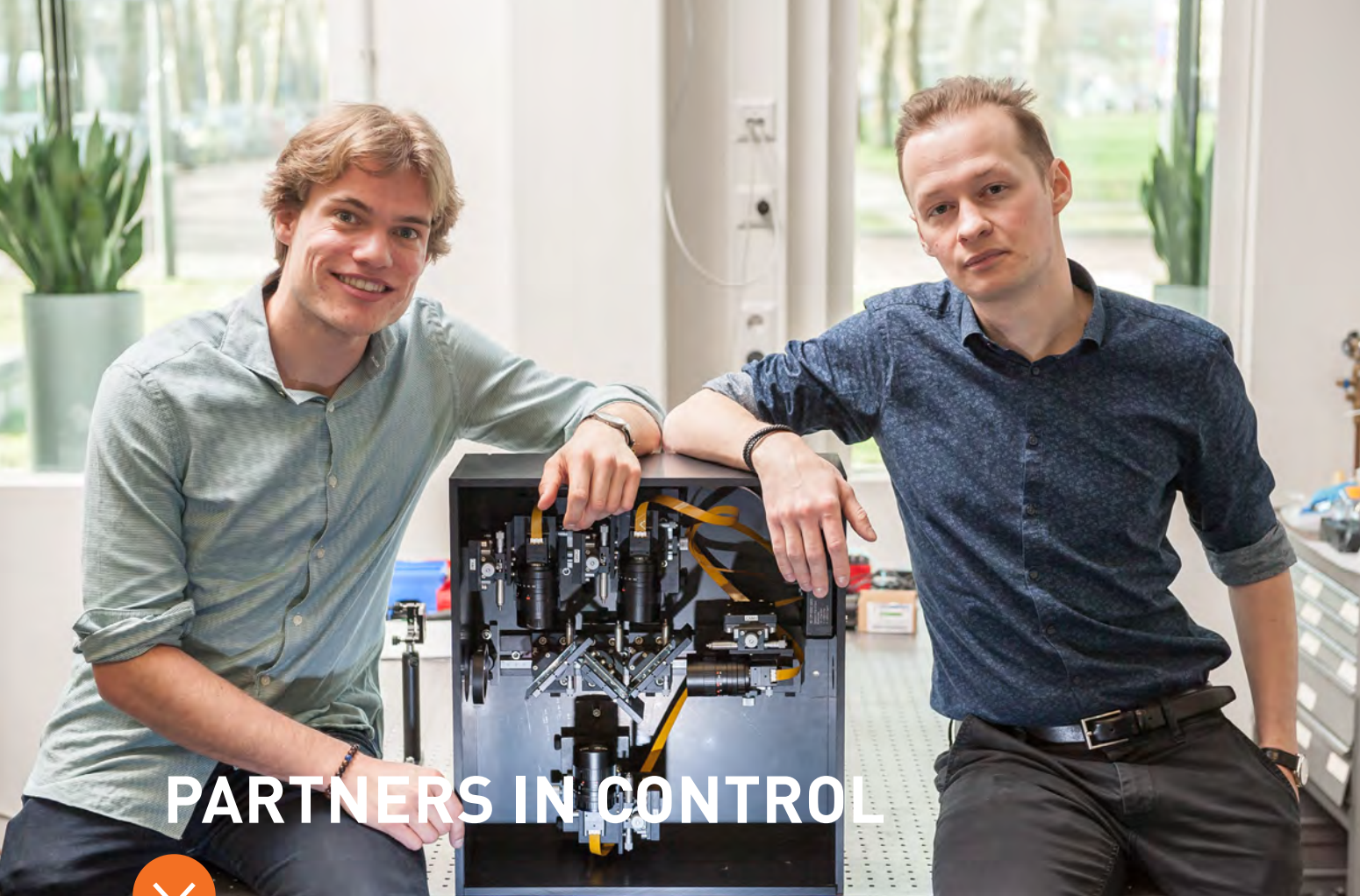
Advanced multispectral camera takes first view of the plasma edge

Operating a fusion reactor is a tricky balance between the need to safely exhaust power via the divertor region and preventing excessive cooling that would disrupt the plasma core. The new MANTIS camera system is developed by DIFFER to study the plasma region in a fusion reactor where this interaction happens. After installation and testing at the Swiss tokamak TCV, MANTIS is now taking experimental data across a range of wavelengths.

Future nuclear fusion reactors aim at sustaining a core plasma temperature of 150 million °C, while engineering limits on their wall materials are about 1500 °C. This creates a challenge to safely exhaust the fusion power in form of the extreme heat and particle fluxes without damaging the plasma facing components. An interesting mechanism to tackle this challenge is plasma detachment. Detachment can balance various atomic and molecular processes to avoid both excessive cooling in the plasma exhaust that would disrupt the plasma core, and insufficient cooling that damages the plasma facing components.



2-D distribution of the hydrogen molecular density in the Pilot-PSI device calculated by Soledge2D-Eirene



PARTNERS IN CONTROL



Timo Ravensbergen and Artur Perek

INTERVIEW - Timo Ravensbergen and Artur Perek

Physicist Artur Perek and mechanical engineer Timo Ravensbergen are so used to working together, that the two PhD candidates even finish each other's sentences.

'To reduce the heat load on the inner wall of the fusion reactor, the plasma is cooled locally. This leads to the formation of a drastically cooled neutral gas,' explains Ravensbergen. 'We aim to actively control the formation and movement of the front between those two states to prevent the core plasma from cooling down.' Perek: 'I use the plasma diagnostic MANTIS to make detailed images of this front, and pass the data - with the accuracy of a Swiss watch - to different parts of Timo's algorithm.'

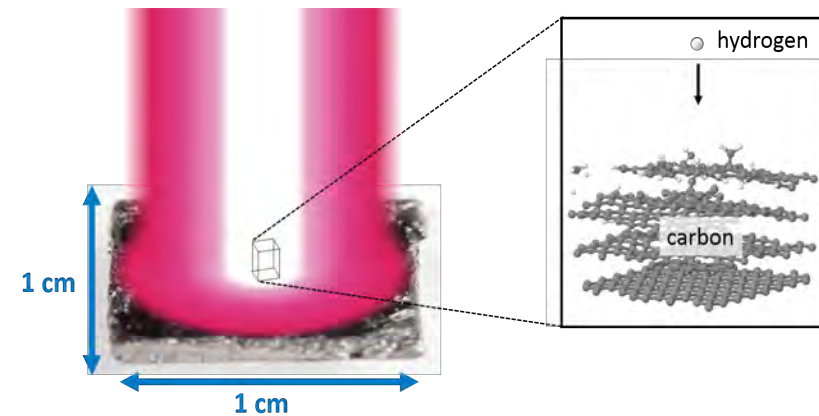
Their multidisciplinary approach pays off, they note. 'The first time we presented our ideas about plasma control, the fusion community was sceptical. But ever since we have shown that it works rather well, everyone is very enthusiastic. We were even allocated significant experimental time on two different machines in Switzerland and the UK.'



The innovative MANTIS camera system will be developed further for applications outside of fusion by spin-off company Chromodynamics, founded by DIFFER post-doc Wouter Vijvers. Chromodynamics will develop high-speed, real-time multispectral imaging systems for medical and industrial applications.

Understanding graphene etching through a million times speed-up

Molecular Dynamics simulations can give great insight into physics at the atomic level, but are typically limited to very small sizes and timescales. Using a novel speedup technique called Collective Variable Hyperdynamics (CVHD), Damien Aussems of the Plasma Material Interactions group was able to incorporate processes on 1 million times longer timescales, revealing that thermal processes are much more important to graphene etching than was previously understood. These simulations reach timescales comparable to those in Magnum-PSI, enabling comparison to experiments with similar fluxes for the first time.



Simulation of the intense plasma-surface interaction region in the centre of the Pilot-PSI linear device. The box under investigation measures 1.2 x 2 x 7 nanometers.

Mechanisms of elementary hydrogen ion-surface interactions during multilayer graphene etching at high surface temperature as a function of flux, Carbon 137, 527-532 (2018)

Spin-out of Remote Handling Study Center

On Tuesday 20 February 2018, DIFFER's Dutch Remote Handling Study Center (RHSC) focused on research on remotely controlled robots spun out to become an independent entity. RHSC was founded within DIFFER with Heemskerk Innovative Technology and developed maintenance techniques for future fusion reactors such as ITER. The spin-out enables RHSC to broaden its scope to include industrial maintenance and even health care.



Front: Cock Heemskerk (HIT) and Wim Koppers





CREATING NEW OPPORTUNITIES FOR RESEARCH

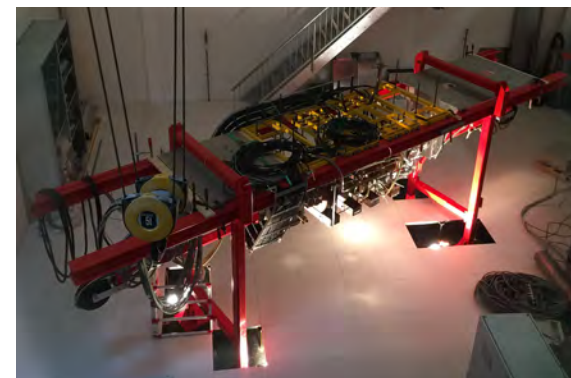
Marc van de Pol

INTERVIEW - Marc van de Pol

"With the upgraded setup Pilot-PSI (Plasma Surface Interaction), we are creating an innovative system to enable groundbreaking research in the field of plasma-surface interaction. That is what motivates me as a technician in a research institute: every day we need to solve challenging technical problems to create systems that meet a need," says research engineer and project leader Marc van de Pol.

The upgraded Pilot-PSI facility is to be the second linear plasma device at DIFFER, and the first to allow for ion beam analysis of how materials change while they are being exposed to extreme plasma conditions in future fusion experiments. "It is an interesting and complex puzzle to find out how we can achieve simultaneous exposure to both the plasma and the ion beam."

"This is the first time I am leading a project of this size and scale. It is a challenge to finish it on time, within budget and according to specifications. So far, we are on track to deliver the first phase of the system in 2019."



Top: Control room UPP; bottom: Upgraded Pilot-PSI

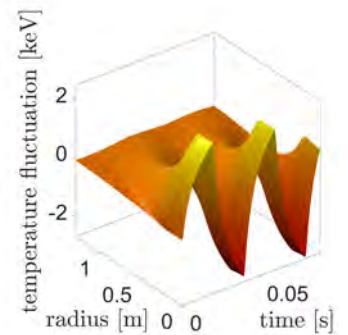
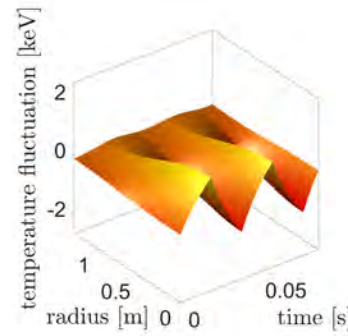


Photo: Matthijs van Berkel at the TU/e campus; Left: Model of the temperature waves that would result from different heat deposition profiles under identical plasma conditions. The top graph fits well with experimental observations, by allowing that the heat source may deposit its power over a wider range than usually assumed. The bottom graph assumes a very localized heat deposition, but then needs to be augmented with complex transport explanations to reproduce the experimentally observed behavior.

Engineering approach simplifies model for plasma heating

In the journal Nuclear Fusion, researcher Matthijs van Berkel shows that a change of perspective can help crack complex problems. Van Berkel studies how heat is transported in fusion plasmas, which is crucial to keeping future fusion reactors at optimal performance.

Analyzing a series of results from the Large Helical Device stellarator LHD, Van Berkel noticed that published claims of complex, non-local non-linear heat transport in the plasma did not lead to the output signal you would

expect from a control engineering perspective. A validation experiment then showed that a much simpler physical model could produce the same results.

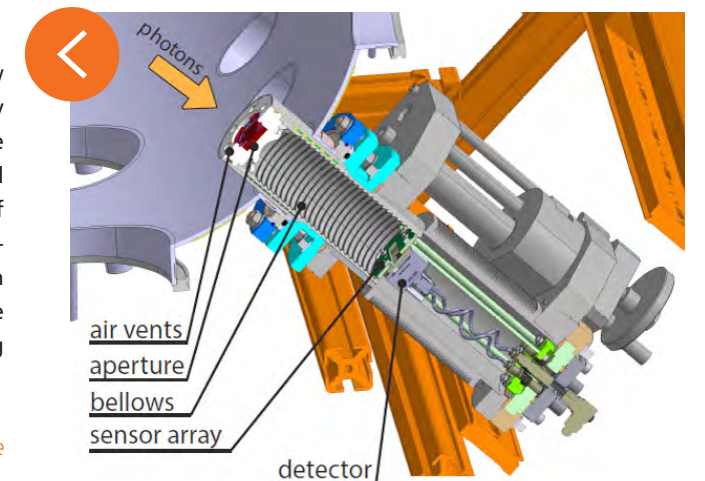
"Physicists often assume a perfect heat source, which dissipates the vast majority of its heat in a designated small volume in the plasma. But I argued that in practice, heat sources are never perfect and parts of the heat can end up in other sections of the plasma. That turned out to be an elegant new view that, we expect, leads to many of the effects that previously were attributed to non-localized transport."

Separation of transport in slow and fast time-scales using modulated heat pulse experiments (hysteresis in flux explained), Nuclear Fusion 58(10), 106042 (2018)

Zooming in on exhaust power

A big question for fusion power exhaust is how much power is radiated close to the wall, especially for evaporated and sputtered particles from these surfaces. To investigate this process, a four channel bolometer was installed to investigate the emission of radiation close to plasma exposed targets in Magnum-PSI, the first time such an instrument has been used in a linear plasma device. The four channels enable the measurements to be made at different points along the beam axis.

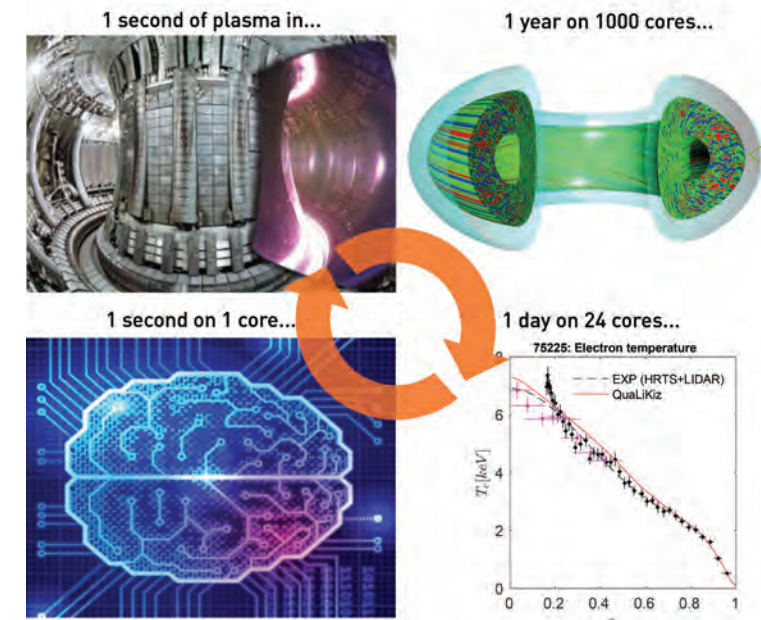
Plasma radiation studies in Magnum-PSI using resistive bolometry, Nuclear Fusion 10, 10 (2018)



A schematic of the bolometry system installed in Magnum-PSI

Blazingly fast fusion plasma simulators enabled by machine learning

Transport in fusion plasmas is dominated by turbulence. Accurate transport prediction is vital for interpreting current fusion experiments, and optimising design of future devices. While the framework of nonlinear gyrokinetics provides high-fidelity predictions of tokamak turbulence, it comes at the cost of extensive calculation time on high-performance supercomputers. Development of validated reduced turbulence models applied within tokamak simulation suites, such as the QuaLiKiz model co-developed at DIFFER, can provide significant speedup of $\times 10^6$. However, these models are still too slow for extensive scenario optimisation and control-oriented applications. Karel van de Plassche from the Integrated Modeling and Transport group applied neural networks to develop a fast surrogate model, by "learning" the QuaLiKiz model based on a database of 300 million experimentally relevant calculations pre-generated on supercomputers. The neural networks reproduce QuaLiKiz predictions $\times 10^6$ faster, a trillion times faster than nonlinear simulations! When integrated in tokamak simulators such as control-oriented RAPTOR, or the integrated modelling suite JINTRAC, we can now simulate a second of JET plasma evolution within several seconds of computation time. This is unprecedented, and opens up a plethora of applications in tokamak optimisation and control.

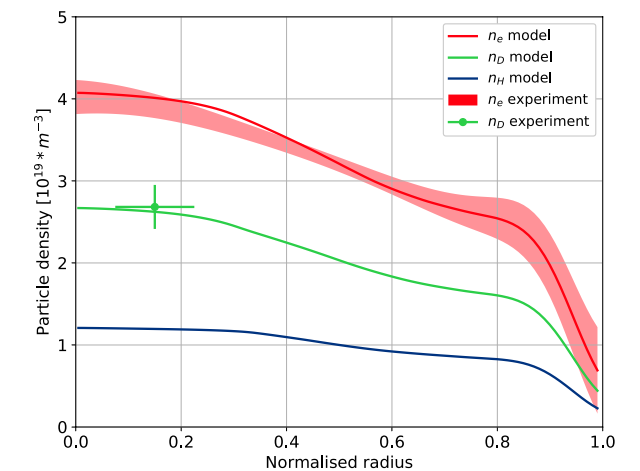


Predicting turbulence in fusion plasmas through a hierarchy of ever faster computer models.

K.L. van de Plassche et al., to be submitted to Nuclear Fusion

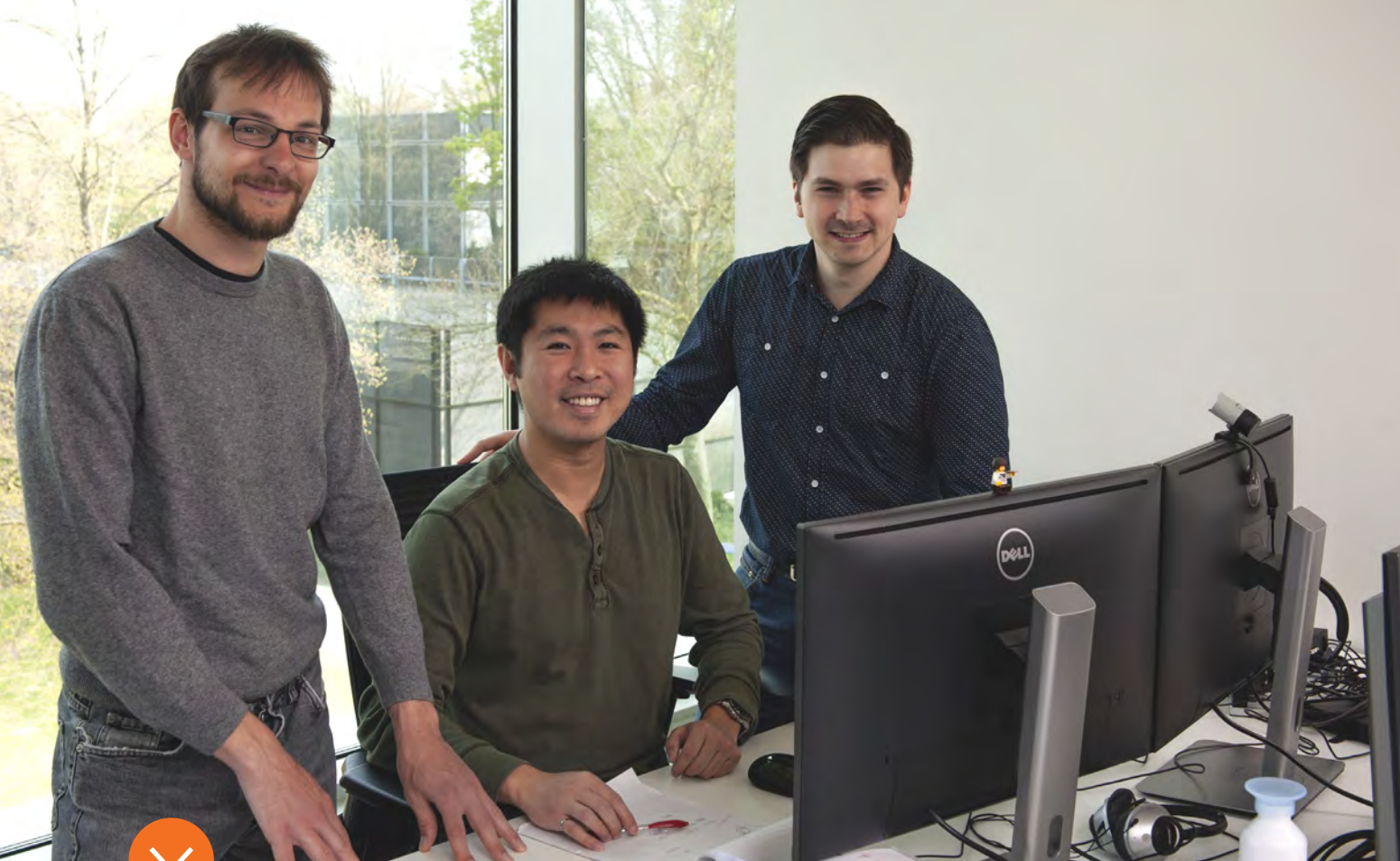
Accurate predictions of multiple-ion turbulent transport at JET

For optimal performance, a fusion reactor plasma must maintain a near equal 50-50% mix of its deuterium (D) and tritium (T) fusion fuel. In addition, a fast response of the fuel mix to modifications in fuelling sources is important for efficient control of the fusion power output. Understanding the turbulent transport of these different plasma ion constituents is important to predict and optimise these processes. Recent experiments at the JET tokamak suggest a fast mixing of hydrogen and deuterium, a proxy for DT-mixed plasmas. Michele Marin in the Integrated Modeling and Transport group performed detailed turbulence modeling to unveil the mechanism responsible for this fast transport of ions. The experiments were then successfully modelled by integrated modelling of the core plasma, using the reduced turbulence model QuaLiKiz, co-developed at DIFFER. This provides confidence in our underlying physics models in new regimes, taking a additional step towards virtual tokamak simulators.



Comparison of modelled and measured densities of particle species throughout a fusion plasma

M. Marin et al., to be submitted to Nuclear Fusion



IMT group members Michele Marin, Aaron Ho and Karel van de Plassche

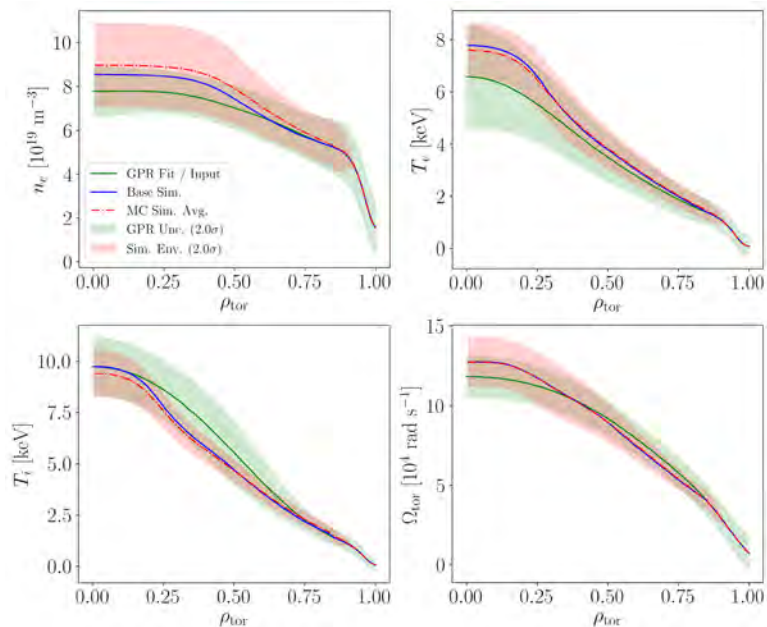
Improved processing of tokamak experimental data

Recent efforts in fusion research has seen a large push towards predictive fusion plasma modelling both for optimising plasma experiments and designing future fusion reactors. To move towards this new frontier, the performance of our models in comparison to

experiments must be checked by rigorous validation, verification, and uncertainty quantification. An advanced statistical algorithm employing Gaussian Process Regression was implemented by DIFFER researcher Aaron Ho from the Integrated Modeling and Transport group to process plasma profiles, such as temperatures and densities as a function of position, in a more general fashion. The results and their estimated uncertainties were then used to improve statistical rigour and significance in model validation and assess any points for improvement. This was showcased in newly developed workflows for the Qualikiz reduced turbulence model, operating within tokamak plasma simulation suites and tested on experimental data from the JET tokamak. These methods also facilitate data mining for machine learning applications, opening up novel and exciting avenues taking advantage of large repositories of experimental data to speed up predictive modelling.

A. Ho et al., accepted by Nuclear Fusion

Validating the predictive QualiKiz reduced turbulence model against experimental data from the JET tokamak



RESEARCH

THEME SOLAR FUELS



Theme leader:

Richard van de Sanden

Research groups: 9

Science staff:

permanent staff 9
post-docs 20
PhD students 24
research engineers 6

Peer reviewed publications 52

Open access publications 35

PhD theses 4

Invited talks 37

Personal grants, prizes, positions:

- ISPT grant on plasma conversion - Mihalis Tsampas
- LIFT Grant - Mihalis Tsampas
- Fontys/TNW best bachelor thesis prize - Ruth Verbroekken
- EPS poster prize - Luca Vialetto
- IKNCV Golden MSc thesis finalist - Ruben Hamans

Industrial collaborations:

NL Alliander, Ampleon, CerPotech, DNV.GL, Fujifilm Research, Gasunie, HyGear, Lumileds, Philips, Philips Lighting, Shell, Stedin, Syngaschem
EU ENGIE (Fr), Evonik, INERATEC, Protemics GmbH (D), Toyota Europe
World Facebook (USA), Sasol (SA)

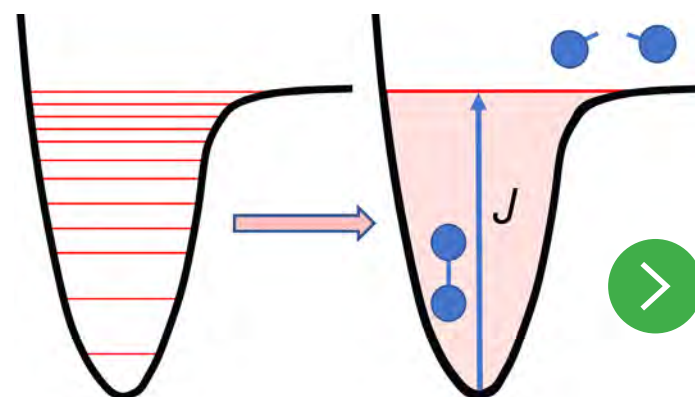


DIFFER's Solar Fuels research directly addresses the challenges posed in the Energy Transition route of the Dutch National Research Agenda (NWA).

Utility companies are looking for solutions that enable them to smoothly match the demand for energy with the intermittent supply from renewable sources like solar and wind energy. The Solar Fuels research at DIFFER explores new ways to efficiently convert and store sustainable energy into high-value chemicals such as fuels and feedstock molecules, by designing and developing novel materials and processes to obtain scalable, efficient and cost-effective systems.

The Solar Fuels research and development program at DIFFER explicitly aims for cost-effective and energy-efficient solutions. Chemical bonds are not only capable of storing high amounts of energy in small volumes, but since they are very stable, there are also perfect candidates for long-term energy storage and long-distance energy transport. Furthermore, DIFFER aims to develop solutions that are based on abundantly available materials. The research focusses on the use of direct or indirect renewable energy to split water into hydrogen and oxygen, and on the reduction of carbon dioxide (CO₂) to carbon monoxide or directly to other products.

More specifically, we focus on plasmolysis, where nonequilibrium plasma is used to efficiently dissociate CO₂; on the artificial leaf approach, where we try to mimic nature by using electrochemical cells to directly convert sunlight into chemical bonds; and on the synthesis, preparation, and characterization of novel (nano) materials for the production of solar fuels and chemicals.



Restating models for the plasma-induced dissociation of CO₂

Defect engineering boosts photocurrent

Hydrogen production from photoelectrochemical (PEC) water splitting is a promising pathway for converting sunlight into chemical fuels. However, efficiency and performance is still too low for rapid commercialization. It is well known that defects play a crucial role in obtaining high performance.

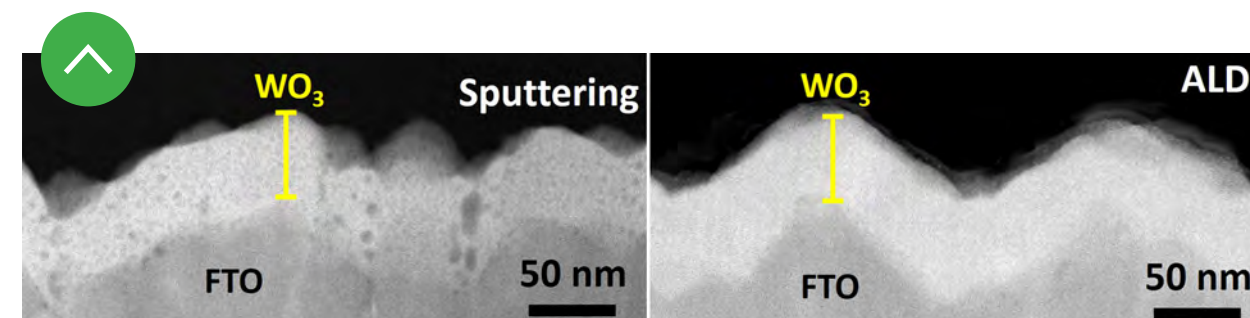
Therefore, PhD student Yihui Zhao from the DIFFER group Electrochemical Materials and Interfaces (EMI) of Anja Bieberle-Hütter investigated the impact of physical and chemical defects on the PEC performance. The work published in ACS Applied Energy Materials was carried out in collaboration with the TU/e and focused on the photoanode material tungsten oxide (WO₃) which is known for its high electron mobility, suitable band-gap, and good chemical stability.

Physical defects, such as micro holes or cracks, were studied by two different deposition techniques: sputtering and atomic layer deposition (ALD). Chemical defects, such as oxygen vacancies, were tailored by the annealing atmosphere, i.e. air, N₂, and O₂. It was found that the physical defects inside

the film increase the resistance for charge transfer and also result in a higher recombination rate which inhibits the photocurrent generation. Chemical defects, in contrast, yield in an increased adsorption of hydroxyl groups on the film surface and enhance the PEC efficiency. Excess amount of chemical defects, however, inhibit the electron transfer and thus decrease the photocurrent.

Hence, deposition techniques and processing parameters enabling the deposition of high quality, defect-free thin films and interfaces are crucial for high performing PEC electrodes. Chemical defects need to be tailored well due to their dual effect on performance. Significant boost in PEC performance with a single material and simple structure was demonstrated.

Physical and Chemical Defects in WO₃ Thin Films and Their Impact on Photoelectrochemical Water Splitting, ACS Applied Energy Materials 11, 5887-5895 (2018)



Cross-section transmission electron microscopy images illustrating physical defects in thin films prepared by different deposition methods: sputtering and atomic Layer Deposition (ALD).

Diffusion theory helps understand how molecules dissociate in plasma

Plasma induced CO₂ dissociation is under widespread investigation as a stepping stone to CO₂-neutral fuels production. Current models for this process are based on the State-to-State approach which is effective but slightly hinders the insight, because it does not limit the number of chemical reactions between different vibrational states. Therefore a complex graph emerges, where each of the many states is connected to several others. Together with Professor Savino Longo from Italy, DIFFER's Computational Plasma

Physics and Chemistry (CPPC) group of Paola Diomedea developed a model which transforms the relation network between different states into a diffusion process like that of ink in water. Moreover, the model offers very fast calculations requiring only the solution of ordinary differential equations. Studies of this type make it possible to identify key parameters and improve the dissociation process.

Vibrational Kinetics in Plasma as a Functional Problem: A Flux-Matching Approach, J. Phys. Chem. A 122, 7918-7923 (2018)



CREATING IMPACT ON MULTIPLE LEVELS



Qin Ong with fellow works council members Bram Wolff and Dennis Ronden

INTERVIEW - Qin Ong

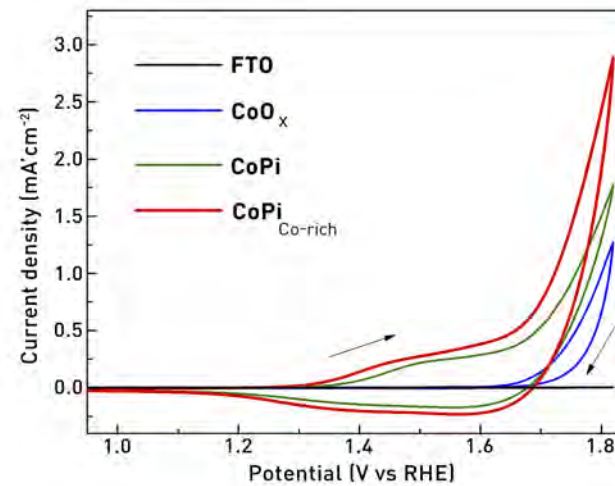
PhD candidate Qin Ong wants to contribute to a sustainable society. "I study the dissociation of carbon dioxide (CO₂) to form carbon monoxide which is an important intermediate to produce hydrocarbon fuels. An efficient way to decompose CO₂ is hypothesized via the vibrational ladder climbing mechanism. I have provided an indirect proof of this mechanism in a mid-infrared laser experiment. At the free-electron laser facility FELIX in Nijmegen, I will study this ladder climbing mechanism in more detail. Ultimately, we aim to use a plasma instead of a laser to decompose CO₂,

since that would be more efficient and significantly cheaper."

In addition to her research, Ong also invests time in the DIFFER Works Council. "It is very instructive to represent my fellow colleagues and to gain insights into the institute's management and governance." During her two-year membership, Ong is involved in updating the Risk Inventory and Evaluation documents and in advocating a diverse community as a member of DIFFER's diversity task force.

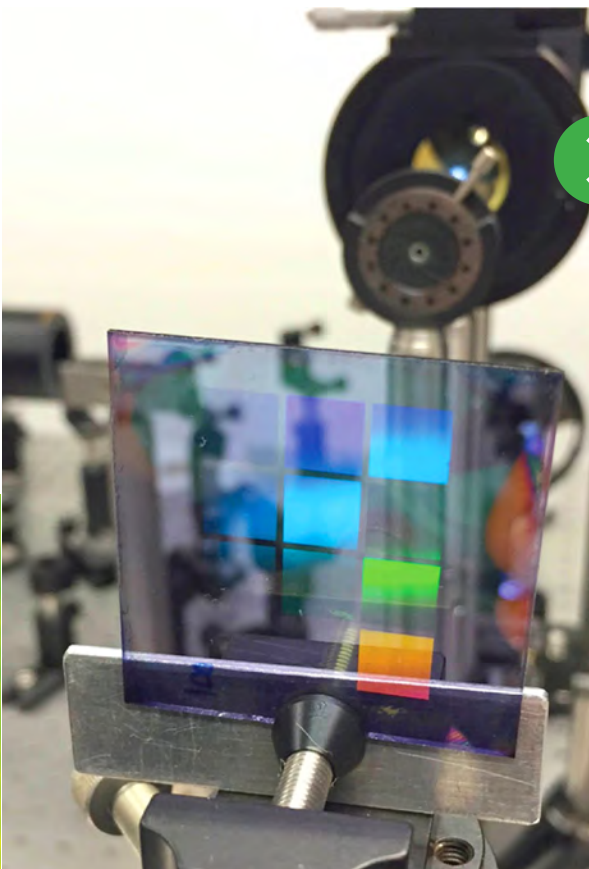
Careful cobalt phosphate deposition boosts water splitting electrolysis

Splitting water into hydrogen and oxygen is a viable approach to store renewable energy in the form of fuels. In the last few decades research has been dedicated to obtaining cost-effective electrocatalysts. In this regard, cobalt based electrocatalysts show the most promising results. So far, the preparation of cobalt phosphate (CoPi) based electrocatalysts is largely limited to (photo)electrodeposition with poor control of the thickness and composition. A higher level of control over material quality can be achieved using atomic layer deposition (ALD).



Using the ALD approach, the CEPEA group of Mihalis Tsampas together with TU/e's PMP group demonstrated that the ratio of cobalt/phosphorus has a direct impact on the activity of the electrocatalyst. A cobalt/phosphorus ratio increase from 1.6 to 1.9 results in over 60% increase in the current density for the oxygen evolution reaction, a notorious bottleneck for water splitting. The ALD cobalt phosphate electrocatalysts now outperform the electrodeposited ones.

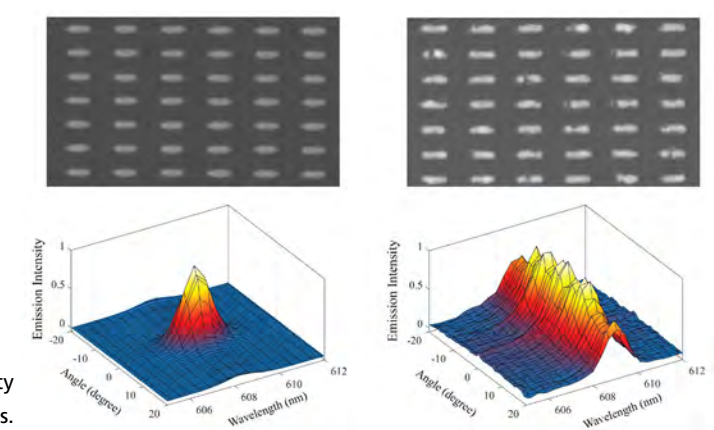
Atomic layer deposition of cobalt phosphate thin films for the oxygen evolution reaction, Electrochemistry Communications 98, 73-77 (2019)



Nanoparticles enable omnidirectional laser

In the very active field of nanoscale lasers, DIFFER-TU/e researchers have discovered a new kind of laser with omnidirectional emission. A laser is usually formed by an optical cavity and an active medium and characterized by its coherence, which makes the emission very intense in defined directions. The nanolaser developed in this research consists of a regular pattern of silver nanoparticles defining the cavity, and that is covered with a polymer and with organic emitting molecules forming the active medium. The nanoparticles deliberately have some degree of imperfection and disorder. The emission from this laser mainly determined by vibrations in the organic molecules and it is surprisingly intense in all directions.

Nonlinear Emission of Molecular Ensembles Strongly Coupled to Plasmonic Lattices with Structural Imperfections, Phys. Rev. Lett. 121, 243904 (2018)



Omnidirectional laser achieves a laser cavity through a grid of silver nanoparticles.

Transferring expertise

Two DIFFER research groups left the Solar Fuels theme in 2018. The successful Photonics for Energy group headed by Jaime Gómez Rivas has decided to join the TU/e to further expand its activities in polaritonic devices, ultrafast spectroscopy, nanophotonics and metamaterials as the Surface Photonics group.

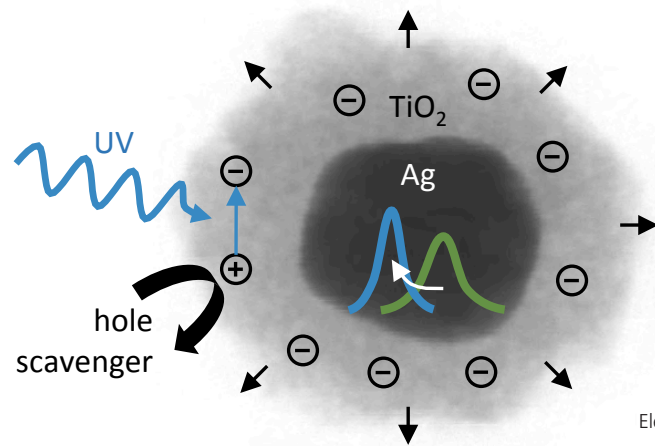
With the graduation of its three PhD students, the group on Atmospheric Plasma Processing of Functional Films successfully completed its Industrial Partnership Programme on plasma-assisted deposition with Fujifilm Research.

TU/e EINDHOVEN UNIVERSITY OF TECHNOLOGY

FUJIFILM

Where have the electrons gone?

Controlling the separation of light-generated charge carriers in semiconductors is fundamental for energy conversion processes. Metal nanoparticles can be used as electron sinks and the charge accumulation can be probed using their plasmon resonances, which are light-driven oscillations of their free electrons. Such resonances, in fact, are extremely sensitive to minor changes in the particle's charge



density. Plasmonic sensing of charge accumulation was initially demonstrated using Ag@TiO₂core@shell nanoparticles: UV irradiation in the presence of hole scavengers led to accumulation of electrons in the metallic cores and a blue-shift of the plasmon resonance. DIFFER researchers Matteo Parente and Andrea Baldi however, together with the Dionne group at Stanford, show that this interpretation of electron storage in metallic nanoparticle is unphysical. Their new interpretation, based on the accumulation of the electrons in the semiconductor, shows how plasmonic nanoparticles can be used to sense and activate chemical processes at the nanoscale.

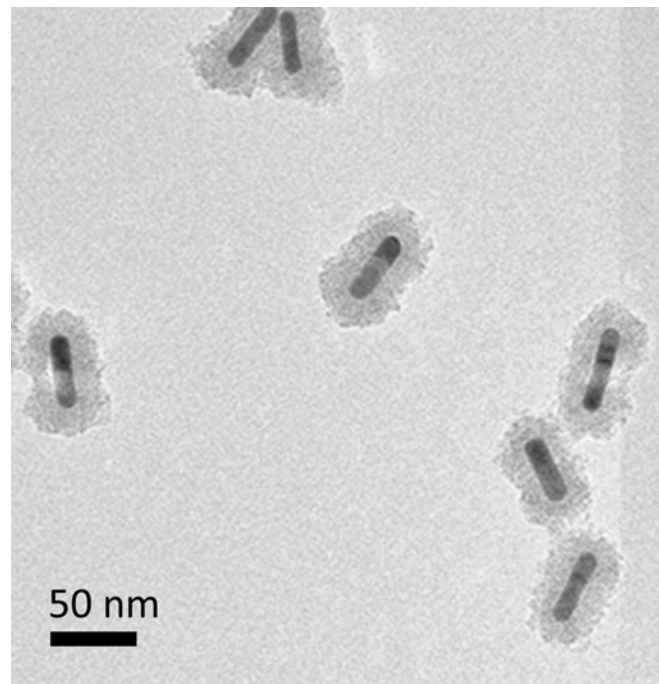
Equilibration of Photogenerated Charge Carriers in Plasmonic Core@Shell Nanoparticles, Journal of Physical Chemistry C 122, 23631–23638 (2018)

Electron accumulation in TiO₂ leads to swelling of the shell and reduced damping of the plasmon resonance.

New electron microscopes to characterize energy materials

DIFFER's research groups in Solar Fuels and Fusion Energy study a wide range of inorganic materials with sizes of the order of 1 nm up to several 1000 nm. To further strengthen the in-house capabilities for materials research the institute acquired and commissioned two electron microscopes in 2018.

The institute's new benchtop scanning electron microscope (SEM) can determine the morphology and composition of photocatalytically or electrochemically active mixed materials. It is one of the first such devices delivered in the Netherlands and combines the convenience of a coffee-machine-size footprint with the resolution performance down to 3 nm of typical cupboard-size SEMs. In addition, a second-hand transmission electron microscope (TEM) enables structural characterization and electron diffraction measurements. The TEM can image materials down to the atomic level with a nominal resolution of 0.2 nanometers. Together with an atomic force microscope (AFM), the new SEM and TEM setups extend the portfolio of characterization tools that are available through a collaboration with Nanolab@TU/e.



TEM image of plasmonic gold nanorods coated with a thin TiO₂ shell.

Sustainable plastics from methane

Making plastics such as polyethylene (used for e.g. plastic bags) from natural gas could help the chemical industry to reach climate goals during the transition phase to a sustainable future. The technology already exists but is too expensive because it involves a detour. A single step process is a long-cherished wish and is subject of investigation in a collaboration between DIFFER, University of Twente and Sasol, financed for 2/3 by the NWO chemical innovation fund and for 1/3 by industrial partner Sasol.

The project is rooted in the combination of plasma chemistry and heterogeneous catalysis. DIFFER developed the diagnostic means to characterize and optimize the plasma methane activation step.

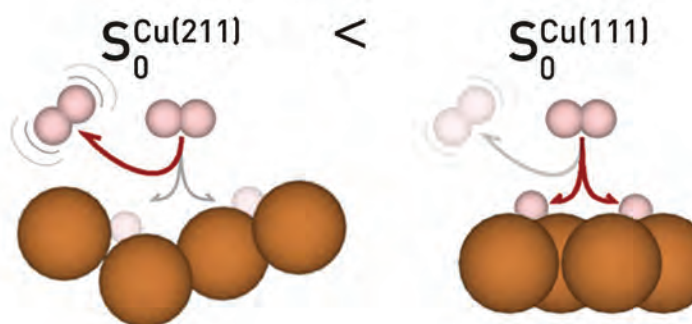
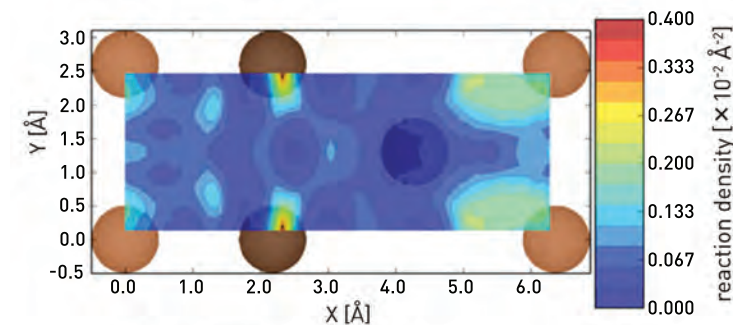


UNIVERSITEIT TWENTE.

This was used to identify how efficient selectively breaking only one bond per methane molecule can be achieved. The University of Twente designs the catalyst that specifically promotes the formation of higher hydrocarbons from methane fragments.

Fundamental insight into structure-sensitive catalyzed reactions

In heterogeneous catalysis, as in real estate, the location is important. Understanding where the optimal reaction sites to promote the chemical reactions are located on a catalyst surface, could lead to better, more efficient production of the majority of human-made chemicals. Computational scientists from DIFFER's Autonomous Energy Materials Discovery group have made a detailed investigation of how complex surface nanostructures, such as the edges and corners of metal surfaces, influence those ideal reaction sites. Together with experimental researchers from Leiden, University they analyzed how hydrogen reacts on stepped copper surfaces. Interestingly, the new results contradicted the general notion that, the edges - such as the steps on the modeled copper surface - would show increased catalytic activity; in fact, flat single-crystal surfaces are found to be more advantageous to dissociate hydrogen molecules.



(Top) lowest reaction barriers as function of the impact sites, (bottom) sticking coefficients, S_0 , are about twice on flat surface to that of on stepped surface.

Anomalous Dependence of the Reactivity on the Presence of Steps: Dissociation of D-2 on Cu(211)), J. Phys. Chem. Lett. 9, 1, 170-175 (2018)



Süleyman Er



BUILD FROM SCRATCH

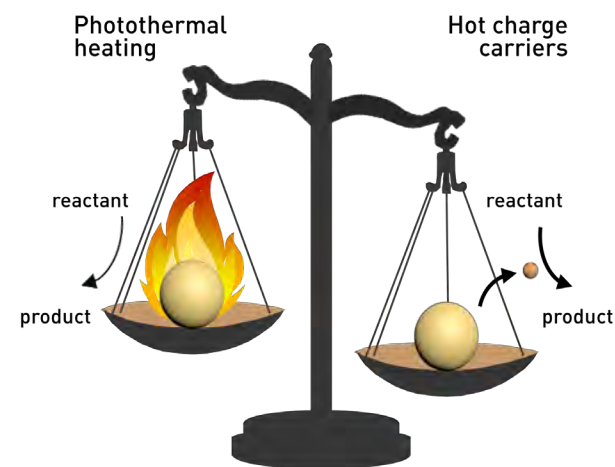
Rifat Kamarudheen

INTERVIEW - Rifat Kamarudheen

PhD candidate Rifat Kamarudheen joined the institute at the same time Andrea Baldi came over to start the group Nanomaterials for Energy Applications. "I could help build up both the group and the lab from scratch. That is an extremely useful experience for when I am starting my own group someday."

His finest scientific hour so far? When he disproved his own intuition. "It is known that light can accelerate chemical reactions. But no-one knew exactly how. We devised an experiment to distinguish between the two most prominent theories, that attribute this acceleration either to heating effects or to hot charge carriers. Since charge carriers are extremely short-lived, we expected thermal effects would explain everything. Imagine our surprise when we found out that in fact the thermal effects are negligible."

Exciting times are ahead, he concludes. "We are now conducting experiments to discard all thermal effects and only use hot carriers to engineer new nanostructures with potential applications in catalysis and energy devices."



Quantifying photothermal and hot charge carrier effects in plasmon driven chemical processes.

Quantifying Photothermal and Hot Charge Carrier Effects in Plasmon-Driven Nanoparticle Syntheses, ACS Nano 12 (8), 8447-8455 (2018)



Collaboration with polytech yields printable electrodes project

Together with Fontys University of Applied Science and the companies Syngaschem and Domicro, DIFFER initiated a research project on the prospects of inkjet printing for the fabrication of electrodes that feature new electrocatalysts for water electrolysis. Knowledge development and transfer aside, this project also showed the strength of the NWO-SIA sponsored DIFFER-Fontys joint lectorate of Peter Thüne. This cooperation aims facilitate and stimulate applied research in the field of Solar Fuels and to allow Fontys students a hands on experience with Solar Fuel research. In 2018 a dozen Fontys students have worked as interns within the DIFFER research groups.



Fabrication and testing of a printed metal-oxide electrode

DIFFER-Fontys lector Peter Thüne



NETWORK BUILDING

WORKING TOGETHER ON ENERGY RESEARCH

Collaboration is key to accelerate the energy transition and reach the world's climate target of limiting global warming to 2 °C at most, and preferably 1.5 °C.

At DIFFER, we invest in an energy research community in the Netherlands and beyond. We focus on connecting the relevant disciplines and actors, from fundamental and applied research, development and prototyping, to enterprises and industry. We strive to foster cross-disciplinary collaborations that will lead to necessary breakthroughs for mid- and long-term sustainable technologies.

ACOS conference on applied computational science

On 10 October 2018, DIFFER welcomed over 150 participants to the annual Applied Computational Science (ACOS) conference, organized by NWO, CCER and Royal Dutch Shell. The goal of ACOS is to bring together the Dutch research community in applied computational science. The conference is intended for both academic and industrial researchers developing and using computational methods to tackle industrial and societal challenges. ACOS aims at sharing and discussing developments in the field whilst building an active and sustainable community in the Netherlands.

The Center for Computational Energy Research (CCER) aims to explore pathways to future energy systems via computational simulations that complement experimental energy research. The center was founded in 2017 as a joint initiative of the Department of Applied Physics of the Eindhoven University of Technology and DIFFER, and comprises researchers from both organizations. With CCER as ACOS co-organizer, the annual conference is well positioned to strengthen the collaboration between computational researchers at DIFFER and at the TU/e.



Over 150 participants attended this year's Applied Computational Science (ACOS) conference

Connecting with Horizon2020

With a project in the Horizon2020 framework, DIFFER is bringing together research and industry in networks for sustainable energy research.

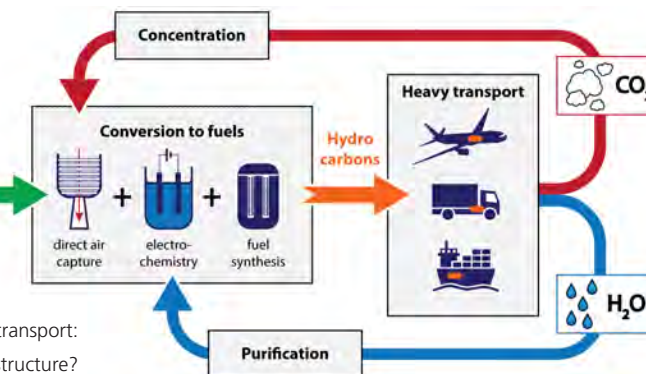
Aviation is a striking example of a sector that is hard to wean off fossil fuels, as batteries, hydrogen and hybrid combinations are limited by their low energy density. The KEROGREEN project is coordinated by DIFFER and aims to develop the production of synthetic kerosene from ambient water and CO₂ instead of fossil resources. Project partners are Karlsruhe Institute for Technology, the Flemish Institute for Technology Research, HyGear, CerPotech and INERATEC.



The Dutch Climate Agreement: advocating energy science

Via the Netherlands Energy Research Alliance NERA, DIFFER is working hard to provide scientific input to the national climate agreement and its mission innovation programmes. This agreement will set out pathways and measures to reach the Dutch CO₂ targets for 2030. Societal and industrial partners were invited to provide input via five sector tables on Electricity, Built Environment, Industry, Agriculture and Land Use, and Mobility.

The science community provided their input at specialized tables, also with an outlook to the 2050 targets. As chair of the NERA Scientific Board, DIFFER director Richard van de Sanden is involved in shaping the innovation challenges on the short and long-term. This ongoing process will lead to the Integral Knowledge and Innovation Agenda of the Climate Agreement that is structured around missions for 2050.



Part of the ECCM concept illustrated for sustainable high-density fuels for heavy transport: what steps are needed to manufacture and integrate clean fuels into infrastructure?



KEROGREEN kick-off meeting participants (www.kerogreen.eu)

Connecting energy, chemistry and high-tech manufacturing

How can researchers and high-tech companies work together to bring about the sustainable production of feedstock molecules and fuels? The committee on Electrochemical Conversion and Materials (ECCM) chaired by DIFFER's Richard van de Sanden takes a nationally coordinated approach in bringing these two worlds together.

The coordinating efforts build on the ECCM advisory report issued in 2017 and have resulted in tenure track positions funded by the national science organization NWO to strengthen the strong electrochemical knowledge base in the Netherlands.

In the future, a national ECCM platform will bring together relevant stakeholders from research, innovation and companies. This process was kick-started with a national ECCM conference that DIFFER organised for participants in the Topsectors High Tech Systems and Materials, Energy and Chemistry. DIFFER already actively promotes the theme Fuelliance in the Province Noord-Brabant and its Brainport Eindhoven region. In line with the ECCM advice, Fuelliance aims to connect sustainable electrochemistry to high-tech, innovative manufacturing companies providing components, equipment and system concepts.

NETWORK ACTIVITIES

Bringing sustainable energy technology from the laboratory to the application phase takes many different parties working together. DIFFER organises this network of science for future energy via events with researchers in academia and industry, polytechnicals and technological institutes.



PHYSICS @VELDHOVEN

Focus sessions "Electrochemical processes in energy applications" (Dr. Anja Bieberle) and "Plasmonics for Chemistry" (Dr. Andrea Baldi) to highlight scientific developments to the Dutch physics and chemistry communities.

- Physics at Veldhoven, January 2018
- NWO CHAINS conference, December 2018

EnergyDays TU/e

BROADEN YOUR VISION ON ENERGY AND CLIMATE

Knowledge sharing with students and professionals on renewable fuels and chemicals.

TU/e - DIFFER Energy Day, March 2018 - 100 participants

HORIZON2020

DIFFER coordinates the H2020 research project KEROGREEN on producing sustainable jet fuels

Kick-off Kerogreen, April 2018 - EU consortium

SCOM 2018

Chairing the international workshop Strong Coupling with Organic Molecules in Eindhoven

SCOM 2018, April 2018 - 125 scientists



Agenda setting in energy storage technologies for the EERA JP Energy Storage

EERA Energy Storage, May 2018 - 50 EU experts

A platform on electrochemical conversion and materials for scientists, researchers, industry and policy makers.

ECCM conference, June 2018 - 200 participants

NERA

Netherlands Energy Research Alliance

Providing a stage to pitch proposals linking to the NWA route Energy Transition

NWA matchmaking, July 2018 - 80 participants

CCER

Center for Computational Energy Research

APPLIED COMPUTATIONAL SCIENCE SYMPOSIUM

OCTOBER 10, 2018

DIFFER EINDHOVEN

Bringing together academic and industrial researchers working in applied computational science

ACOS symposium, October 2018 - 150 participants

OUTREACH

KNOWLEDGE TRANSFER TO SOCIETY

One of DIFFER's goals is transferring knowledge to society at large. The institute welcomes young talent for research projects in the upper levels of high school, in the bachelor and master phase, and as technical apprentices. DIFFER also runs a strong outreach program to the general public, either via the media or directly in the form of open days.

Media reach

Broadcast items	2
Newspaper articles	12
Magazine publications	9
Online publications	13
[www.differ.nl/news/media-clippings]	

Reach of events and activities

Open day	350
Science stand ITER open day	700
Higher education students	60
High school students	62



Lab tour: Dutch Physics Olympiad

On 14 June 2018 DIFFER organised a visit for the 25 finalists in the Dutch Physics Olympiad. The students visited diverse laboratories such as the Magnum-PSI facility for plasma surface interactions, and the nanomaterials for energy applications chemical laboratory.

Solar Fuels special in Dutch physics magazine

Can we turn renewable energy into clean and CO₂-neutral fuels? In the *zonnebrandstoffen* special of the Dutch Physics Journal NTVN, DIFFER researchers showed how they aim to turn water, CO₂, sunlight and wind into fuels for a sustainable society.



Videos present DIFFER's research on Youtube

Together with NWO, researchers Anja Bieberle and Thomas Morgan created two videos for the general public about DIFFER's energy research. Scan the QR to see the video.



<https://www.youtube.com/watch?v=aN2K0HJeuRA>



Fusion Road Show at ITER open doors day



Showing that a magnetic field can shape a plasma at a distance (Photo: ITER)

How do you start people out on a tour across the vast ITER worksite? To provide a fusion crash course, ITER invited DIFFER communicator Gieljan de Vries to present a special edition of the Fusion Road Show during its open doors day on May 26th. And so, with the world's biggest fusion project in the background, visitors stood mesmerized by a kitchen microwave. What's cooking is not their lunch, but a glowing ball of plasma: all to



Capturing a microwave plasma in a pyrex beaker (Photo: ITER)

explain that capturing the ITER plasma will take specially tailored materials and magnetic fields. Over 700 people visited the ITER open doors day.



OPEN HOUSE DAY 2018

DIFFER's annual open day is the institute's main event to talk with the general public about how our research can help create a sustainable future. The 2018 Dutch Science Weekend saw 350 visitors come to DIFFER to discuss future energy solutions with the experts, participate in workshops, get hands-on experience with splitting water into hydrogen fuel, or visit the many labs and outreach talks. With visitors giving an average appreciation score of 8.3 out of 10, the open day clearly was a great success.



FACTS & FIGURES

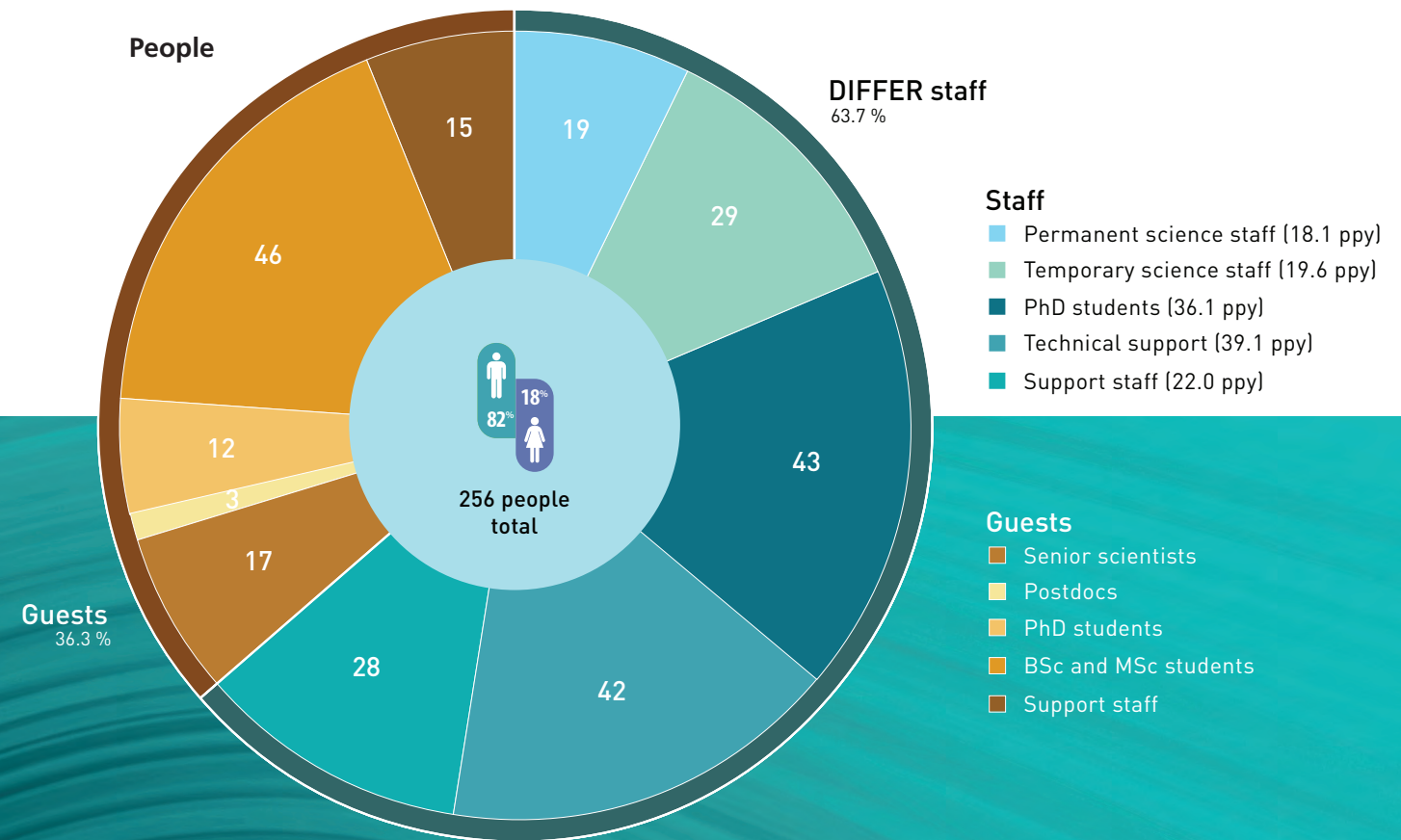
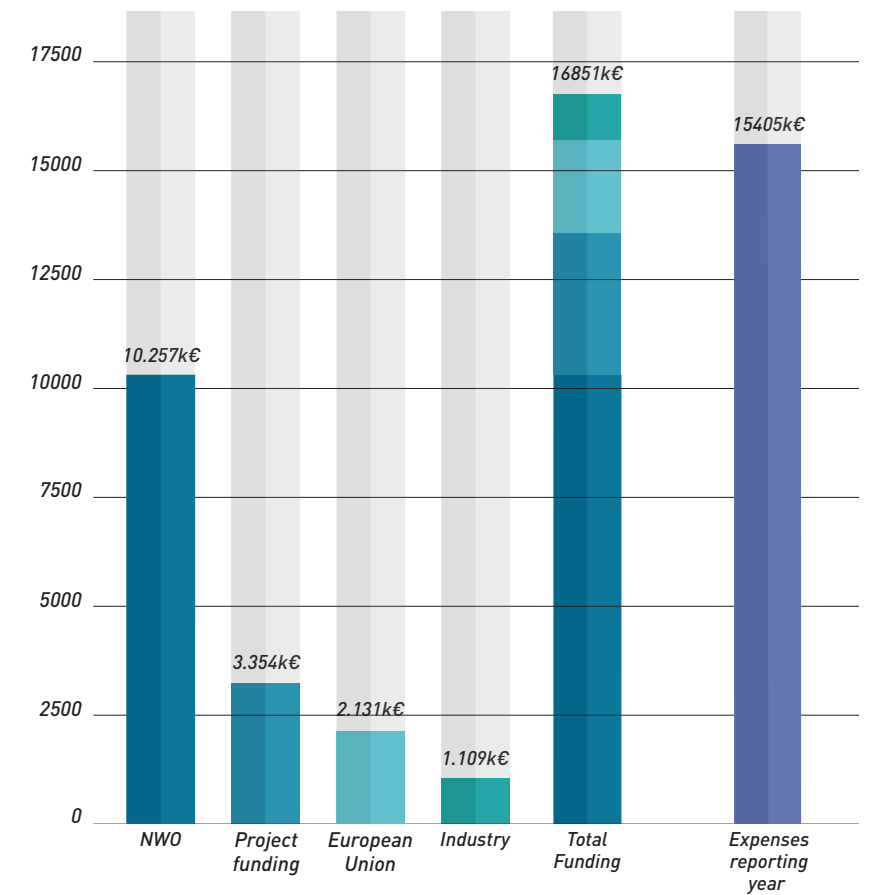
Output 2018



Organizational chart



Funding and expenses 2018



Committees

Management Team

M.C.M. van de Sanden (institute director; theme leader Solar Fuels)

W.R. Koppers (institute manager)

M.R. de Baar (theme leader Fusion Energy)

Scientific Advisory Committee

C. Bourdelle (Commissariat à l'énergie atomique et aux énergies alternatives)

U. Fantz (Augsburg University)

R. van de Krol (Helmholtz - Zentrum Berlin)

D. Lincot (Institut de Recherche et Développement sur l'Energie)

E.B. Stechel (Arizona State University)

H.G.C. Werij (Delft University of Technology) (*chair*)

Works Council

B.S.Q. Elzendoorn (*chair up to October 2018*)

A. Ho

G. Kaas (*chair as from October 2018*)

D.M.S. Ronden

F.J. van Amerongen

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