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# De Oosterpoort, Groningen
# Friday, 7 April 2017

## Focus Session: Physics & Energy

**Programme:**

- Anitha Immaneni (Shell): Enhanced Experimentation in Shell
- Roberta Croce (VU): Different carotenoid conformations have distinct functions in light harvesting regulation in plants
- Fokko Mulder (TUD): Efficient electricity storage with a battolyser, an integrated Ni–Fe battery and electrolyser
- Elizabeth von Hauff (VU): New approaches to understand electrical transport in molecular and nanostructured semiconductors

Session leaders: Giuseppe Portale & Maria Antonietta Loi (RUG)

**Abstracts:**

Anitha Immaneni (Shell): Enhanced Experimentation in Shell
Enhanced Experimentation (EE) uses a combined set of tools including: high-throughput experimentation(miniaturization and parallelization); robotics and automation; advanced analytical methods; computer modeling, and data management tools, with the aim of significantly speeding up R&D, engineering and related technical processes. These tools – upon successful derisking – improve R&D productivity, and shorten our time-to-market.

One characteristic feature of the EE platform is our extensive external focus: More than two-thirds of our projects have been developed together with external parties, experts in different aspects of EE. This has resulted not only in great speed of delivery, but also in bringing in valuable technological solutions from other industries (like Pharma, Food & Paints, Steel manufacturing) for the benefit of several Shell businesses. Few successful projects: development of new chemicals for Enhanced Oil Recovery, Alternates to animal testing, commercial products from hydrocarbon waste, functional coatings for energy efficiency .

In this talk, I will present some such examples.

Roberta Croce (VU): Different carotenoid conformations have distinct functions in light harvesting regulation in plants
To avoid photodamage in high light conditions, plants regulate the amount of excitation energy in the membrane at the level of their antennae, pigment-protein complexes known as the light-harvesting complexes (LHCs). It has been proposed that the dissipation of the energy absorbed in excess is induced by protein conformational changes of individual LHCs that modulate the interactions between pigments. However the exact quenching mechanism(s) remains unclear. We have studied the mechanism of quenching in LHCs that bind a single carotenoid species and are constitutively in a dissipative conformation. Via femtosecond spectroscopy we resolved a number of carotenoid dark states characterized by distinct spectra and lifetimes, suggesting that the carotenoid is bound to the complex in different conformations. Some of those states act as excitation energy donors for the chlorophylls while others act as acceptors and are thus responsible for the observed quenching. Via *in*

*silico* analysis, we show that structural changes of carotenoids are expected to occur in the LHC protein domains on the lumenal side of the photosynthetic membrane, where acidification is known to trigger photoprotection *in vivo*. We, therefore, propose that structural changes of LHCs affect the conformation of the carotenoids thus permitting access to dark states that can act either as energy donors or as quenchers.

Fokko Mulder (TUD): Efficient electricity storage with a battolyser, an integrated Ni–Fe battery and electrolyser

Grid scale electricity storage on daily and seasonal time scales is required to accommodate increasing amounts of renewable electricity from wind and solar power. We have developed for the first time an integrated battery-electrolyser ('battolyser') that efficiently stores electricity as a nickel–iron battery and can split water into hydrogen and oxygen as an alkaline electrolyser.[1] During charge insertion the $Ni(OH)_2$ and $Fe(OH)_2$ electrodes form nanostructured NiOOH and reduced Fe, which subsequently act as efficient oxygen and hydrogen evolution catalysts respectively. The charged electrodes use all excess electricity for efficient electrolysis, while they can be discharged at any time to provide electricity when needed. The energy density and efficiency of the battery electrodes is competitive with high energy density batteries for static storage. The electrolysis reaches competitive efficiency and switchability without using noble metals. Our results demonstrate a remarkable constant and a high overall energy efficiency (80–90%), enhanced electrode storage density, fast current switching capabilities, and a general stable performance during intensive long term tests. The integration leads to a device which can be used constantly with a high capacity factor: as a battery for storage on very short to daily timescales, and as an electrolyser when the battery is full, providing fuel for long term storage. The battolyser may enable efficient and robust short-term electricity storage and long-term electricity storage through production of hydrogen as a fuel and feedstock within a single, scalable, abundant element based device.

**Reference**

[1] F.M. Mulder, B.M.H. Weninger, J. Middelkoop, F.G.B. Ooms and H. Schreuders,
Energy and Environmental Science, in press (2017), Hot article, DOI: 10.1039/c6ee02923j

Elizabeth von Hauff (VU): New approaches to understand electrical transport in molecular and nanostructured semiconductors

Organic and nanostructured semiconductors offer many advantages for energy conversion, saving and storage applications. However, poor electrical properties, particularly low carrier mobilities, trapping and recombination phenomena, are a critical limitation for real opto-electronic applications. Surprisingly, carrier transport is still not well-understood in these systems, making it difficult to develop design strategies for high performance applications. There is an increasing number of reports indicating the importance of considering the effects of phonon modes and molecular vibrations on the evolution of excited states in this class of materials. New experimental strategies are urgently needed to correlate dynamic relationships between semiconductor structure and electronic transport. I will present our current work on combining vibrational and impedance spectroscopies to elucidate electron-phonon interactions in organic and nanostructured semiconducting films. I will demonstrate this approach with results from organic semiconductors, and give examples of extending it towards nanostructured and hybrid photovoltaic systems.