## **Newsletter**

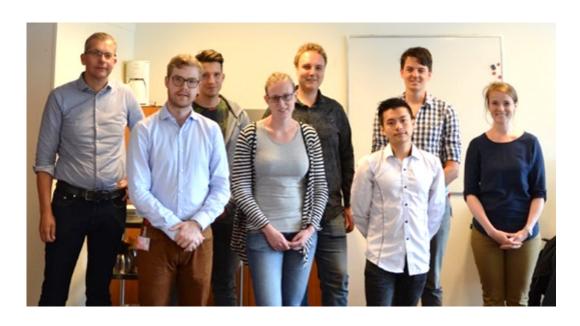
Stratingh Institute for Chemistry

June 2018

#### Strating Award for the best-written colloquium of 2017

On Thursday May 17, the winner of the Strating Award for the best-written colloquium of 2017 was announced. After an introduction on the history of this prestigious prize by Prof. Gerard Roelfes, the three nominees that were selected by the selection committee were announced. The committee, consisting of 2 staff members (Marthe Walvoort and Johannes Klein) and 2 PhD students (Balint Fridrich and Steven Wan), ranked the 18 colloquia on criteria like critical analysis and clarity of writing.

The prize for the third place went to **Jasper Paauwe** for his colloquium entitled "Chitin as an alternative feedstock for fossil resources based chemicals". The runner up of this year's Strating Award was **Linda Eijsink**, with the colloquium entitled "Why is shea butter yellow?". And the winner of the 2017 Strating Award is **Ruben Andringa**, with the colloquium entitled "Radical cascades as key-step in natural product synthesis". The colloquium was a stunning showcase of the application of radical, it was well-written and with clear figures. The award ceremony was followed by coffee and cake for the members of the Stratingh Institute and a lunch for the members of the H.J. Backer foundation, the selection committee and the three nominees of the Strating prize.



#### Ruth Dorel is awarded the Josep Castells Award

Ruth Dorel, a Post Doc in the Feringa Group won the Josep Castells Award for the best PhD Thesis in 2017. Her thesis is titled: "New Annulation Strategies: From Polycyclic Aromatic Hydrocarbons to Natural Products"

The Josep Castells Award is given annually by the Catalan Section of the Spanish Royal Society of Chemistry (RSEQ-CAT) and it recognizes the best PhD thesis.

#### Prof. Edwin Otten is awarded Teacher of the Year for Chemistry

The Teacher of the Year for Chemistry 2018 was awarded to Prof. Edwin Otten. The Teacher of the Year event is organized yearly by the Programme Committee for Chemistry and Chemical Engineering. Students vote for their favorite teachers in either Chemistry or Chemical Engineering. The top three lecturers in each category then go on to compete against each other in the finale by giving a 10 minute presentation that showcases their teaching abilities.

# Bálint Fridrich is awareded the poster prize of the 14<sup>th</sup> International Conference on Renewable Resources and Biorefineries

Bálint Fridrich from the Barta Group won the poster prize of the RRB 14 Conference with the poster titled: "The efficient catalytic conversion of short chain oxygenates derived from ABE fermentation to jet fuel range alkanes". More than 230 people participated from 33 countries and close to 100 oral presentations and 87 posters were presented. The conference took place in Ghent, Belgium from 30th of May - 1st June and was mainly focused on efficient utilization of biomass.



Many Congratulations to Michael Lerch from the Feringa Group for receiving his doctorate degree with Cum Laude



#### Highlights by Prof. dr. Jan B.F.N.Engberts

This is the final issue of the Highlights before the summer holiday. I wish all my readers a most pleasant and refreshing holiday to stimulate your scientific creativity when you start your research again!

Wiebe and Waldvogel, together with four colleagues from the Max Planck Graduate Center in Mainz and the Johannes Gutenberg University, also in Mainz, published a large review (86 pages!) under the title "Electrifying Organic Synthesis" in Angew. Chem.Int.Ed. The argued that the direct synthetic organic use of electricity is at the moment experiencing a renaissance. The technology is now extended to novel as well as traditional concepts leading to broader applications. A large number of these valuable applications are discussed in some detail. Since only electrons are employed as reagents, the production of reagent waste can be efficiently avoided.

Wiebe, A., Gieshoff, T., Möhle, S., Rodrigo, E., Zirbes, M., Waldvogel, S.R., Angew.Chem.Int.Ed., 2018, DOI 10.1002/anie 201711060.

A remarkable paper was published in Science by Kang-Kuen Ni and six colleagues at Harvard University, USA. For the first time two atoms (Na and Cs) have been combined into a dipolar molecule, which is a new type of qubit, the smallest unit of quantum information which has great importance for the future of quantum computing. The two individual laser-cooled atoms are trapped in separate optical tweezers and are then merged into one optical dipole trap. Photo-association then forms an exited-state NaCs molecule. The tightly trapped ultracold sample of atoms leads to the discovery of previously unseen resonances at about the molecular dissociation threshold and the measurement of collision rates. It is argued that many further developments are possible, including the synthesis of designer molecules for qubits.

Liu, L.R., Hood, J.D., Yu, Y., Zhang, J.T., Hutzler, N.R., Rosenband, T., Ni, K-K., Science 2018, DOI 10.1126/science.aar7797.

Itami and two coworkers (Nagoya University, Japan) published the first palladium-catalyzed esterification of carboxylic acids with aryl iodides. The ligand (1,3-bis((pentafluorophenyl)methyl) imidazole-2-ylidene) (IBn<sup>F</sup>) significantly accelerated the aryl-O bond-forming esterification. Particularly electron-rich aryl iodides showed good reactivity, also in a gram-scale synthesis. Also sterically hindered aryl iodides were well-tolerated and afforded aryl esters in varying to good yields (up to 86%). Mechanistic studies and a more detailed investigation of the ligand effect are ongoing in the laboratory.

Kitano, H., Ito, H., Itami, K., Org. Lett. 2018, DOI 10.1021/acs.orglett.8b00775.

Manganese-catalyzed benzylic C(sp³) amination for late stage functionalization was examined by White and three coworkers from the Roger Adams Laboratory in the University of Illinois, Urbana, USA. The direct installation of nitrogen into C-H bonds of complex molecules is an important process because it can change the chemical and biological properties of the compound. The paper reports a base-metal-catalyzed intermolecular benzylic C-H amination that proceeds with high levels of reactivity, site selectivity and functional group tolerance. A [MnIII(ClPc)] was prepared in a one step, scalable reaction from abundant and sustainable commercial starting materials. The C-H amination catalyzed by this compound demonstrates high site selectivity based on steric and electronic

differentiation. These properties and several other advantages make the catalyst uniquely useful for late-stage functionalization of bioactive molecules and natural products. Mechanistic studies suggest that C-H cleavage is the rate-determining step (the primary kinetic isotope effect is about 2.5). The key intermediate is most likely an electrophilic metallonitrene. It is anticipated that the mechanistic features will allow a tunable control of site selectivity when the reactivity is increased for intermolecular amination of other C(sp³)-H bond types.

Clark, J.R., Feng, K., Sookezian, A., White, M.C., Nature Chem. 2018, DOI 10.1038/s41557-018-0020-0.

Segler, from the Westfälische Wilhelms-Universität in Münster, with one colleague from the same University and one from Shanghai University in China, made a detailed comparison of the efficiency of traditional retrosynthetic routes and computer-aided retrosynthesis based upon Monte Carlo tree search and symbolic artificial intelligence (AI). The deep neural networks were trained on essentially all single-step synthetic processes ever published, about 12.4 million of them. The results obtained using a "deep learning" computer program gave blueprints for the sequences of reactions needed to create organic molecules, including drug compounds. It was clear that the synthetic routes based on the new software are a milestone and make organic chemistry more efficient since more time is left for real intellectual challenges.

However, a number of scientists, including the famous science blogger Derek Lowe, have another opinion and say that the computer-assisted synthetic planning (CASP) rests on the idea that intellectual tasks might be categorized as automatable grunt work.

Segler, M.H.S., Preus, M., Waller, M.P., Nature, 2018, DOI 10.1038/nature25978.

Ben Feringa, with eight coworkers from three Research Institutes at the University of Groningen and one from the DWI-Leibniz Institute in Aachen, Germany and one from RWTH Aachen University, Germany, published the first study in which a molecular motor was employed to control the secondary structure of DNA. It is one of the first cases in which a molecular motor was used under physiological conditions for regulating DNA hybridization, which is a key biological process. Externally regulated biomolecules have recently been recognized as highly attractive tools in nanosciences. The present study shows that molecular motors offer highly useful and precise methods for photoregulation, as a result of their multistage switching cycle. The measured lower melting temperature of 6 °C for an 8 bp hairpin indicates the success of the method for the design of potent molecular motor-backbone linkers. The molecular motor can be applied under physiological conditions to control the secondary structure of DNA and further studies of the regulation of key biological processes by molecular motors will certainly be found.

Lubbe, A.S., Liu, Q., Smith, S.J., de Vries, J.W., Kistemaker, J.C.M., de Vries, A.H., Faustino, I., Meng, Z., Szymanski, W., Herrmann, A., Feringa, B.L., J.Am.Chem.Soc. 2018, DOI 10.1021/jacs.7b09476.

Jan Engberts

#### New appointments:







M.attia Lenti—PhD Barta Group

Dr . Martin D. Witte has been appointed Associate Professor

### Werkbespreking: Thursday morning 8.30 hrs, room 5111.0080

Jun 21st: Gang Ye, "Conjugated Polymers with Ionic, Water-Soluble Backbones"

Jun 28th : Gongbao Wang

## Tuesday June 26th Nanosymposium 2018

Nanosymposium is an yearly event, that concludes short research projects of Nanoscience first year students. This year it takes place on June 26th, 9 am to 5 pm at Nijenborgh 4, room 5111.0022 and the guest speaker is Prof. Albert Polman from AMOLF "Light management and the dream of photovoltaic energy for 0.01 €/kWh"

for more information as well as to sign up for free lunch, please visit <u>nanosymposium.nl</u>

#### **PhD Defences**

Luuk Kortekaas from Browne Group will defend his thesis on the 25-06-2018 at 11 am Andrew Kovalchuk from Chiechi Group will defend his thesis on the 29-06-2018 at 12:45 pm

If you have items for the next issue of this Newsletter, please send an e mail to the Stratingh Institute office: Stratingh@rug.nl