university of groningen

Newsletter

Stratingh Institute for Chemistry

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February 2016

Kees Hummelen listed, for the third year in a row, in the Thomson Reuters Highly Cited Researchers list.

Every year upwards of 9 million scientists and scholars publish their findings in academic journals, producing papers that, according to some estimates, likely number in excess of 2 million.

With such prodigious output, the task of qualifying the value of each piece of work is challenging. Nevertheless, the research community, publishers, academic administrators and others seek such clarification, beyond means such as who commands the highest salaries, biggest laboratories or office shelves with the most awards.

One strategy, steering clear of the marginal factors noted above, is to concentrate on the research papers themselves – specifically, the extent to which they have assisted, inspired or challenged other researchers. Papers meeting this standard earn a clear distinction when other authors explicitly footnote, or cite, the reports in their subsequent work. A paper that other authors have frequently cited has quantifiably proved itself to be significant.

Extending this logic provides a clear avenue to seek out authors who have consistently produced papers which have, in turn, won peer approval in the form of high citation counts.

This approach is embodied in the Thomson Reuters Highly Cited Researchers, a searchable compendium covering the main areas of science and the social sciences, representing the researchers who, in their respective fields, have contributed markedly high numbers of top-cited papers.

Ben Feringa awarded August Wilhem von Hofmann Denkmunze

The German Chemical Society (Gesellschaft Deutscher Chemiker) has awarded Prof. Ben Feringaof the Stratingh Institute for Chemistry with the August-Wilhem-von-Hofmann-Denkmünze in recognition of his ground-breaking research on dynamic molecular systems, catalysis and stereochemistry. Feringa will receive the award at the 6th European Chemistry Congress in Sevilla, Spain on September 11th, 2016.

Anna Hirsch to receive the "Prix d'encouragement á la recherche en chimie thérapeutique"

To promote excellence, but also to support young researchers at the dawn of their careers, the French Medicinal Chemistry Society ("Société de Chimie Thérapeutique", S.C.T.) provides each year a prestigious prize entitled "Prix d'Encouragement à la Recherche en Chimie Thérapeutique".

This prize is sponsored by "Institut de Recherche Servier", and is devoted to junior European scientists. It rewards an outstanding young researcher, no older than 36, for his research contributions in "Drug Discovery Chemistry" (chemical biology, chemoinformatics, structure-activity relationship studies, ADMET, imaging, physical chemistry, biolabeling and diagnostic tools, drug vectorization, nanotechnologies, natural products, structural biology, synthetic methodology, etc...).

This prize may be attributed to one or several young scientists.

This year, the prize was awarded to Anna Hirsch and Dr M. Montés and it consists of a 3,000 euros grant (which will be divided between the two laureates) and consists of an invitation to give a lecture during the upcoming "23rd Young Research Fellows Meeting" to be held in Lille (15-17 February 2016).

Anna Hirsch is awarded a LIFT-project grant for 285000 Euro

The NWO Innovation Fund Chemistry has awarded eight LIFT projects between university researchers and companies. NWO Chemical Sciences contributes a total of 1.5 million euros to the various projects and businesses match 0.5 million euros. LIFT is a new public-private partnership form that was introduced in 2015 . In a LIFT project involves at least one company and one research institute both working in chemical research.

Dr. Anna Hirsch (RUG), Dr . Matthew Groves (RUG), Dr . Gudrun Lange (Bayer CropScience): **On the way to innovative antibiotics and herbicides Antibiotic.** Resistance to herbicide is currently a serious problem. The researchers will design new molecules that inhibit an essential enzyme for the growth of pathogenic bacteria and weeds in a specific way . To do this, they first go to elucidate the structure of the enzyme, after which the rational design of new inhibitors will be used. Ultimately, the drugs can be developed to better antibiotic or herbicide with a completely new mechanism of action.

Sijbren Otto and the Origin of Life

How can life originate from a lifeless chemical soup? This question has puzzled scientists since Darwin's 'Origin of species'. Stratingh Institute chemistry professor Sijbren Otto studies 'chemical evolution' to see if self-organization and autocatalysis will provide the answer. His research group previously developed self-replicating molecules—molecules that can make copies of themselves—and have now observed diversification in replicator mutants. They found that if you start with one ancestral set of replicator mutants, a second set will branch off spontaneously. This means that ecological diversity as encountered in biology may well have its roots at the molecular level. The results were published on Jan. 4, 2016, in Nature Chemistry.

Prof Otto was also interviewed by national television (EenVandaag - NPO) here.

More information:Jan W. Sadownik, Elio Mattia, Piotr Nowak and Sijbren Otto: Diversification of self-replicating molecules. Nature Chemistry, Advanced Online Publication Jan. 4, 2016, DOI: 10.1038/nchem.2419

NWO ECHO grant for Prof. Syuzanna Harutyunyan

Prof. Harutyunyan has been awarded a €260.000 ECHO grant from NWO (the Netherlands Organisation for Scientific Research) to further develop a groundbreaking method for the catalytic, asymmetric synthesis of chiral C-tertiary amines. The novel strategy relies on one-pot alkylation/aza-Brook-rearrangement/carbanion trapping techniques, and promises to afford these important organic, chiral molecules in an efficient, catalytic manner.

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

First of all, all good wishes for my readers for a healthy, happy, and creative New Year!

- I like to start with two developments in fundamental science. Swiss and American scientists (Piazza et al.) have for the first time been able to observe simultaneously light both as a particle and as a wave. Of course we know that light exhibits a wave-particle duality, but imaging this dual behavior simultaneously is really a breakhrough. *Piazza, L., Lummen, T.T.A., Quinonez, E., Murooka, Y., Reed, B.W., Barwick, B., Carbone, F., Nature Comm. 2015, DOI 10.1038/ncomms7407.*
- Secondly, in a recent paper in Nature, Castelvecchi asks the question (and many people before him): "Is string theory science?" He reports a workshop at the Maximillian University at Munich where both leading theoretical scientists and philosophers expressed quite different opinions. Some of them argued that "if a theory is sufficiently elegant and explanatory, it need not be tested experimentally". Others, however, stressed that strings are at the moment too small to be detected (smaller than the Planck-length) and that a theory based on strings is at best speculative. No agreement was obtained during the meeting! *Castelvecchi, D., Nature 2015, 528, 446-447.*
- (-)-Hymenosetin is a fungal metabolite with several biological activities including some promising ones against gram-positive bacteria. Chemists in Mainz and Kaiserlautern, Germany, have developed a general strategy for the total synthesis of this complex molecule in quite a number of steps. The stereochemistry of the rather unusual diastereomer was investigated by circular dichroism in the IR and UV/VIS frequency range. *Kauhl, U., Andernach, L., Weck, S., Sandjo, L.P., Jacob, S., Thines, E., Opatz, T., J.Org.Chem. 2016, 81, 215-228.*
- Aspects of a fundamental theory of the living world have been discussed in a brief paper by Gabriel Popkin. He emphasized particularly the complex movements of biomolecules ("active matter") and the factors determining these processes in biological cells thereby taking energy from their environment. As he puts it: "From flocking birds to swarming molecules, we are seeking to understand active matter". He argues that further insights demand scientists who are at the cutting edge of both physics and biology. *Popkin, G., Nature, 2016, 529, 16-18.*
- Recently there has been great interest in non-fullerene acceptors as potential alternatives to fullerene derivatives in bulk heterojunction organic solar cells. But their power conversion efficiencies (PCEs) are still not sufficiently high. In a joint project of Chinese, South-Korean and American laboratories a novel perylene bisimide acceptor has now been developed, in which selenium atoms were introduced into the perylene core. Using a wide-band-gap polymer as the donor, a high PCE (8.4 %) and a high fill factor were accomplished for solution -processed non-fullerene solar cells. The authors predict an excellent future for these types of materials. *Meng, D., Sun, D., Zhong, C., Liu, T., Fan, B., Huo, L., Li, Y., Jiang, W., Choi, H., Kim, T., Kim, J.Y., Sun, Y., Wang, Z., Heeger, A.J., J.Am.Chem.Soc., 2016, DOI 10.1021/jacs.5b11149.*
- Researchers at Queens Univ., Belfast, UK, the Nat. Univ. of Cuyo, Argentina, the Univ. of Liverpool, UK, the Univ. of Kiel, Germany and Univ. Blaise Pascal, Aubière, France, argue that materials combining the proper-

ties of fluidity and permanent porosity will possess useful technological advantages. However, the second factor has sofar not been associated with conventional liquids. These rather unique liquids have now been obtained for the first time. The concentration of unoccupied cages (diameter ca. 5Å) can be about 500 times greater than that in other molecular solutions that contain cavities. The unifying design principle for these materials is the avoidance of functional groups that can penetrate into the molecular cage cavities. *Giri, N., Del Popolo, M.G., Melaugh, G., Greenaway, R.L., Rätzke, K., Koschine, T., Pison, L., Costa Gomes, M.F., Cooper, A.I., James, S.L., Nature 2015, 527, 216-221.*

- Bert Meijer (Univ. of Techn., Eindhoven) and three colleagues from MIT, Cambridge, Mass., USA have written an interesting review (170 references!) in which they discuss the properties of a number of rationally designed supramolecular biomaterials and their application in drug delivery, tissue engineering, regenerative medicine and immunology. An important issue is the reversible nature of supramolecular interactions. As a result, such biomaterials can sense and respond to physiological cues, or can mimic the structural and functional aspects of biological signalling.The results that are discussed illustrate a broad utility for the design of highly controllable and functional materials for biomedical applications. An advance into clinical practice is predicted involving the treatment of diseases and a thus-far unrealized therapeutic impact. *Webber, M.J., Appel, E.A., Meijer, E.W., Langer, R., Nature Materials 2016, 15, 13-26.*
- A rather unexpected effect was found by scientists at two Universities in New Orleans, USA. Using isothermal titration calorimetry in combination with quantum and molecular dynamics calculations, they demonstrated that relatively soft anions (like the perchlorate and iodide anion) have a clear affinity for hydrophobic concavities. Anion binding can be affected without complete desolvation. The affinity of 26 monovalent sodium salts was investigated for one cavitand at pH 11.5 in water and binding occurred for 18 anions. These are important results and the authors suggest that many anions are most likely able to bind to proteins. *Sokkalingam, P., Shraberg, J., Rick, S.W., Gibb, B.C., J.Am.Chem.Soc., 2016, DOI 10.1021/jacs.5b10937.*
- Finally, I like to draw your attention to an important development. As discussed in a Perspective in Science (Kühlbrandt) and in three Special Features in Nature Methods (Eisenstein, Nogales and Glaeser) there is a recent "resolution revolution" in cryo-electron microscopy. Structures of large macromolecules, including proteins, can now been obtained at near-atomic resolution. Both an advance in detector technology (particularly in the camera) and an advance in image processing are responsible for the present breakthrough. In the future it is not anymore necessary to crystallize large complexes and large proteins, an exciting development! *Kühlbrandt, W., Science 2014, 343,1443-1444; Eisenstein, M.,Nature Methods 2016, 13, 19-22; Nogales, E., Nature Methods 2016, 13, 2427. Glaeser, R.M., Nature Methods, 2016, 13, 28-32.*

Jan Engberts

PhD Defences

Friday, February 5th

@ 14:30 Claudia Poloni will defend her PhD thesis. **Title:** "Peptides in Motion". Promotor: Prof. dr. B.L. Feringa, Co-promotor: Dr. W.C.Szymanski

@ 16:15 Sébastien Perdriau will defend his PhD thesis. **Title:** "New catalytic reactions for the conversion of alkenes". Promotores: Prof. dr. J.G. de Vries, Prof. Dr. H.J. Heeres, Co-promotor: Dr. E. Otten

Friday, February 12th

@ 12:45 Milon Mondal will defend his PhD thesis. **Title:** "Dynamic combinatorial chemistry and protein-templated click chemistry in medicinal chemistry". Promotores: Prof. A. K. H. Hirsch Prof. A. J. Minnaard

Monday, February22nd

@ 11:00 Johanne Penafiel will defend her PhD thesis. **Title:** "Alkaline earth organometallic compounds in homogeneous catalysis". Promotor: Prof. S. Harder

@ 12:45 Harmen Zijlstra will defend his PhD thesis. **Title:** "Mysterious MAO: Towards a Better Structural Understanding of Methylalumoxane and the Development of Well-Defined Alumoxanes". Promotor: Prof. S. Harder

New appointments

Bin Liu

As of 1/11/2015

PhD—Group Otto

Dusan Kolarski

As of 1/1/2016

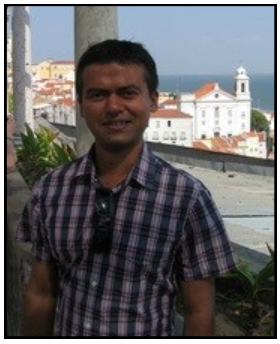
PhD—Group Feringa

Kaja Sitkowska

As of 1/1/2016

PhD—Group Feringa

Lectures



Prof. Dr. Biprajit Sarka
Institut für Chemie und Biochemie, Freie Universität Berlin
Title: Metal Complexes of Mesoionic Carbenes: Redox Non-Innocence and Electrocatalysis
Day: Tuesday, February 9th, 2016
Room: 5111.0080
Time: 16:00
Contact: Wesley Browne (w.r.browne@rug.nl)

Prof. Ruben Martin
ISIQ, Tarragona, Spain
Title: **to be announced**
Day: Tuesday, February 23trd, 2016
Room: 5111.0080
Time: 16:00

Werkbespreking: Thursday morning 8.30 hrs, room 5111.0080

February 4th—Matea Vlatkovic (PhD Feringa): "Dynamic control of chiral space"

February 11th— Andrii Kovalchuk (PhD Hummelen): "Controlling electron charge transport through Self-Assembled Monolayers with organic synthesis"

February 18th—Michael Lerch (PhD Feringa): "Emerging Molecular Photoswitches: Synthetic Methods and Applications"

February 25th—Sureshbabu Guduguntla (PhD Feringa): "Cu-catalyzed asymmetric allylic arylation with organolithium reagents: Synthesis of tertiary and quaternary stereocenters"

March 3rd—Francesco Mecozzi (PhD Browne): "Selective oxidation of alkenes and vicinal diols to acyloins with H2O2 in multistep one-pot reactions using a simple Mn catalyst"

Due to the large amount of PhDs finishing their contract this year it appears more difficult for master students to present their work. For the coming period the master students will present in afternoon symposia instead of the Thursday morning. **The first Stratingh Master Symposium is at 15:00 o'clock on the 16th of February in room 5111.0080** (standard Thursday morning room). The speakers will be:

1) **Reinder de Vries** (Msc Roelfes)
"Synthesis of N4Py Derivatives Containing Targeting Groups for Tumor Cells"
2) **Jorn Steen** (Msc Browne)
"Exploring the properties and applications of redox-responsive ferrocene and carbazole-containing compounds"
3) **Linda Eijsink** (Msc Otten)
"Nitrile activation by a Ruthenium PNN pincer complex"

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