university of groningen

Newsletter

Stratingh Institute for Chemistry

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February 2013

Sijbren Otto is awarded a VICI grant

Towards Darwinian evolution with fully synthetic molecules.

Biological systems exist by virtue of continuous processes of synthesis and degradation. At essentially all levels of biology there is a dynamic balance between formation and decay; between life and death. Ironically, without decay and death there would be no biology. The VICI grant was awarded to learn how to operate synthetic chemical systems in the same continuous synthesis/degradation regime as is commonplace in biology. Mastering these principles and applying these to molecular networks of self-replicating molecules should then enable the development of fully synthetic systems capable of undergoing Darwinian evolution. Such systems would pave the way to the development of de-novo life.

Ben Feringa is awarded the Marie Curie Medal

Ben Feringa has been awarded the Marie Curie Medal, the highest honor awarded annually by the Polish Chemical Society for chemist working outside Poland, given for the outstanding achievements in the field. The medal will be presented in September on a yearly meeting of the Polish Chemical Society. Previous laureates of this medal, awarded since 1996, include Prof. Philip Kocieński (UK), Prof. Christian Reichardt (Germany) and Prof. Krzysztof Matyjaszewski (USA).

Introducing Katalin Barta

Katalin Barta studied chemistry at ELTE Budapest where her master's thesis focused on fluorous biphase chemistry and alternative solvents in the group of Prof. Istvan T. Horvath. Her PhD thesis in the group of Prof. Walter Leitner, at the RWTH-Aachen, concentrated on asymmetric catalysis. She was a post-doctoral researcher in the group of Prof. Peter Ford at the University of California, Santa Barbara where she co-developed efficient methodologies for the catalytic conversion of woody biomass. After, she worked at the Center of Green Chemistry at Yale University, led by Prof. Paul Anastas, as associate research scientist. She joined the Stratingh Institute on February 1st, as assistant professor in Green Chemistry and Catalysis. Her research will focus on developing sustainable chemical processes with emphasis on the catalytic conversion of biomass.

Introducing Tineke Kalter-Meuken

Hello, my name is Tineke. If you cannot pronounce this, just call me Tina. I used to work as a purchaser, account manager in sales and as the secretary for a CEO. I started at RuG this January as the secretary of Ben Feringa and his group. These are my office hours: Monday, Wednesday & Thursday, Tuesday afternoon & Friday morning. Family: happily married to Edwin. We have two adult sons called Bennett and Lester. I admire: the intellect of Fibonacci, the voice of Annie Lennox and the creativity of Jim Henson. I enjoy: playing lego with my grandson Jayden, walking my dogs, visiting theatre and opera and of course holidays in la bella Italia. I like at lot: British comedians like Rhod Gilbert and Michael McIntyre. I am addicted to: reading lots and lots of books, mainly by writers as James Rollins, Ruth Rendell and Erich Maria Remarque. I am fascinated by: the returning patterns in human behaviour. Dislike: rain and dirt. Major dislike: dishonesty and lazy people. Short term goal: visit Rome and also visit the Louvre. Long term goal: to be a good person in as many aspects of life as possible.

Introducing Martin Witte

Martin Witte studied chemistry at Leiden University where he did his Master's thesis in the Bio-organic synthesis group of Prof. Jacques van Boom. He performed a research internship at Stanford University in the group of Prof. Matthew Bogyo before returning to Leiden University to do his Ph.D. in the group of Prof. Gijsbert van der Marel and Prof. Herman Overkleeft. After a postdoctoral period in the same group, he joined the group of Prof. Hidde Ploegh at the Whitehead Institute for biomedical research as a postdoctoral fellow. He joined the Stratingh Institute as assistant professor in Chemical Biology on January 1st, 2013. His research will focus on the development of activity-based probes for previously untargeted enzymes (including sulfatases and sulfotransferases) and on the development of protein labeling techniques.

New personnel advisor for the Stratingh Institute for Chemistry

From January 1st, 2013 the new personnell advisor for the Stratingh institute is:

Ms Marlies Beuving
Working days: ma, di, do, vr
HR Advies Zernike kamer 5161.05.30
050 363 93 03
m.beuving@rug.nl

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

Perhaps one the most remarkable papers in the past six weeks is a report by German physicists who claimed that they have found ultracold quantum gases at absolute temperatures of about -2 degrees Kelvin! So far we have learned that nothing can be colder than T = 0, at this temperature classical particles are at rest. However, using a highly sophisticated experimental approach, involving the use of a small cloud of 11.000 potassium atoms and an optical lattice of laser rays, a negative temperature state for motional degrees of freedom has been created. Applications for such negative temperature states are being considered. Most likely the paper will induce a lot of discussion. *S. Braun, J.P. Ronzheimer, M.Schreiber, S.S. Hodgman, T. Rom, I Bloch, U. Schneider, Science 2013, 339, 52-55. Comments: L.D. Carr, Science 2013, 339, 42-43.*

Cross-coupling between two heteroarenes can be carried out using a Cu(OAc)2-mediated dehydrogenative process in the absence of any other additive. Evidence was obtained for a formal Cu (II) to Cu(0) route by convergent disproportionation of the copper mediator. Unsymmetrical biheteroarenes with structural motives of substantial utility in organic synthesis can be obtained in a concise and green synthetic protocol. The isolated yields are between 64 and 89%. *Z. Mao, Z. Wang, Z. Xu, F. Huang, Z. Yu, R. Wang, Org. Lett. 2012, 14, 3854-3857.*

In a previous report I have already drawn attention to halogen bonding, a type of non-covalent, attractive interactions that has been rather overlooked for a long time in the literature. Although it may be important in many areas of chemistry, including organic chemistry, it has particular importance in crystal engineering. The state of the art and its practice has now been reviewed by scientists of the University of Milan. *P. Metrangolo, G. Resnati, Crystal Growth and Design, 2012, 12, 5835-5838.*

"The Enterprise of Synthesis: From Concept to Practice" is the title of a retrospective account of natural product synthesis adopting the Chiral Synthon Approach. It is spanning about fifty years of research activities by Stephen Hanessian. In his own words: "it is highlighting the interplay between the eye and the mind's eye", with synthesis planning discussed in terms of visual relational and visual reflexive thinking modalities. The review covers a large variety of approaches to efficient synthesis of natural products. *S. Hanessian, J.Org.Chem. 2012, 77, 6657-6688.*

A team of organic chemists of the University of Illinois at Urbana-Champaign, USA, has shown that site-selective functionalizations of complex small molecules can be tuned by simply modifying the electronic nature of the reagents. The success of this strategy can be explained in terms of the Hammond postulate since electronic tuning to a more product-like transition state amplifies site-discriminating interactions between a reagent and its substrate. In this way a minimally site-selective acylation reaction can be transformed into a highly selective and preparatively useful one. A number of examples are given. *B.C. Wilcock, B.E. Uno, G.L. Bromann, M.J. Clark, T.M. Anderson, M.D. Burke, Nature Chemistry, 2012, 4, 996-1003.*

An important issue to be mastered in the development of high-energy rechargeable lithium-air batteries is the reversible reduction and evolution of oxygen. A leap forward has now been created by two scientists from the University of Nankai, Tianjin, China, who report the synthesis of a pyrochlore catalyst that benefits from a mesoporous structure and oxygen deficiencies. Some of the reasons why porosity is important is the requirement for void space for efficient mass and charge transport, and also because of the need for a phase interface on which redox reactions can take place. *F. Cheng, J. Chen, Nature Chemistry, 2012, 4, 962-963.*

Quantum chemical effects in organic chemistry are important and well known. Kinetic isotope effects and tunneling are obvious examples. More recently it has been found that the unique features of quantum mechanics are involved in gaining a biological advantage. These effects go beyond trivial quantum effects and may include harnessing quantum coherence on physiologically

important timescales. The latest results have been reviewed by Lambert and Nori and their coworkers. *N. Lambert, Y-N. Chen, Y-C. Cheng, C-M. Li, G.Y. Chen, Nature Physics 2013, 9, 10-18.*

Azaboradibenzo[6]helicene is a novel semiconductor material possessing helical chirality. Hatakeyama and his coworkers prepared the compound via a tandem bora-Friedel-Crafts-type reaction and showed that it can assume mirror image left-handed and right-handed stereochemical structures. Rather unexpectedly, carrier inversion between the racemate (displaying p-type semiconductivity) and the single enantiomer (displaying n-type semiconductivity) was observed. This carrier inversion is apparently caused by different packing of enantiomeric compounds as induced by helical homochirality. *T. Hatakeyama, S. Hashimoto, T. Oba, M. Nakamura, J.Am.Chem.Soc. 2012, 134, 19600-19603.*

Dihydroneopterin aldolase (DHNA), an enzyme involved in folate biosynthesis, is a promising drug target for the bacterium that causes tuberculosis. Czekster and Blanchard, from the Albert Einstein College of Medicin (New York), found that DHNA efficiently catalyzes three different reactions and generates five distinct products. No metals or cofactors are required. This versatility most likely contributes to its function in bacteria. Important information was obtained about the plasticity required from a catalyst that has high substrate specificity while being capable of utilizing two distinct epimers with the same efficiency to generate five distinct products. *C.M. Czekster, J.S. Blanchard, J.Am.Chem.Soc. 2012, 134, 19758-19771.*

My final report is as astonishing as the first one. Ben-Amotz and coworkers have shed fresh light on hydrophobic hydration, the layers of water surrounding hydrophobic solutes in water. Detailed knowledge about these hydration layers is of utmost importance for an adequate understanding of hydrophobic interactions, one of the most important types of intermolecular interactions in biochemical systems and, in fact, in all aqueous systems. Since the 1940s, different theories have been proposed: increases in “water-structure”, a preference for tangentional hydration, dominant exclusive volume effects, and our insights benefitted from both increasingly sensitive and reliable experimental and computational approaches. Ben-Amotz et al. have employed polarized, isotopic and temperature-dependent Raman scattering measurements with multivariate curve resolution (Raman-MCR). It was possible to explore hydrophobic hydration by mapping the vibrational spectroscopic features arising from the hydrophobic hydration shells of linear alcohols ranging from methanol to heptanol. In short, at low temperatures the waters in these shells possess a greater tetrahedral order and fewer weak hydrogen bonds than the surrounding bulk water. This structure disappears with increasing temperature and is then, for hydrophobic chains longer than about 1 nm, replaced by a more disordered structure with weaker hydrogen bonds than those in bulk water. The importance of these findings has been summarized by Huib Bakker. *J.G. Davis, K.P. Gierszal, P. Wang, D. Ben-Amotz, Nature 2012, 491, 582-585. H.J. Bakker, Nature 2012, 491, 533-535.*

Jan Engberts

Invited lectures

Prof Steven Bell
Queen's University, Belfast
Title: **Improving the Function of Nanoparticles and Nanostructured Materials by Controlling their Surface Properties**
Day: Tuesday, **February 12th**, 2013
Room: **5111.0022**
Time: **10:00**

Prof Wittko Francke
University of Hamburg
Title: **Semiochemicals: Structural principles, evolution, and ecological aspects**
Day: Thursday, **February 14th**, 2013
Room: **5161.0105**
Time: **16:00**

Prof Stefan Hecht
Humboldt University Berlin
Title: **Designing Functional Molecular Nanostructures: From Solution to Surface Confinement**
Day: Thursday, **February 28th**, 2013
Room: **5118.-156**
Time: **16:00**

New Personnel

- **Tineke Kaltar – Meuken— as of January 1st** secretary for the groep Syntetic Organic Chemistry
- **Martin Witte, Assistant Professor**—as of January 1st in the Bio-Organic Chemistry group
- **Katalin Barta, Assistant Professor**—as of February 1st in the Syntetic Organic Chemistry group

Werkbespreking: Thursday morning 8.30 hrs, room 5111.0080

February 7th— J. Bos "Enantioselective Artificial Metalloenzymes by Creation of a Novel Active Site at the Protein Dimer Interface"

February 14th—A. Rizzo "Synthetic efforts towards Auto-OrganoCatalytic reactions; Proline and Dihydroisoquinoline based systems"

February 21st—T. Pijper "Properties and switching behavior of a dithienylethene-tripod structure"

February 28th- M. Colomb-Delsuc "Peptide Self-Replication Driven by Self-Assembly"

March 7th—M. Mondal "Structure-based drug design exploiting dynamic combinatorial chemistry to identify novel inhibitors for endothiapepsin"

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