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Molecular Functional Materials

The Spring Meeting of the Swiss Chemical Society, March 10th, 2006, Department of Chemistry, University of Fribourg

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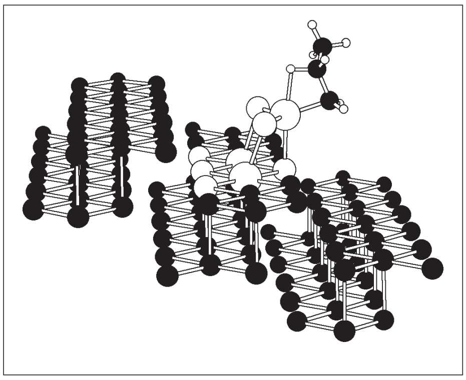
Abstract: The 2006 Spring Meeting of the Swiss Chemical Society was held at the University of Fribourg on March 10, 2006. The one-day symposium was dedicated to recent advances in Molecular Functional Materials. The four speakers, Tom Ziegler, Dante Gatteschi, Andrew Holmes and J. Fraser Stoddart covered a wide range of modern functionalized material research.

Keywords: Computational design · Light emitting diodes · Molecular magnets · Nano Meccano · Polymerization catalysts

The Spring Meeting of the Swiss Chemical Society took place in Fribourg on March 10, 2006. The organizing committee, comprised of *Martin Albrecht*, *Peter Belser,* and *Claude Daul*, chose the general title, 'Molecular Functional Materials', for this one-day symposium. This orientation corresponds to one of the main research topics ('Matter and Life') of the Faculty of Science at the University of Fribourg.

The first lecture of the 2006 Spring meeting, entitled 'Polymerization Catalysts by Computational Design', was given by ***Tom Ziegler*** (University of Calgary). Olefin polymerization is one of the most important industrial processes in which transition metal catalysts play a key role. In this process monomers with an olefinic double bond are stitched together into long polymers with single carbon–carbon bonds.

The first polymerization catalysts were developed by Ziegler and Natta (1953–1955). They were heterogeneous; consisting of $TiCl_4$ supported on silica or $MgCl_2$ with the additives – bases and tri-methyl aluminium. The first part of the talk illustrated the combination of quantum mechanical methods and statistical approaches, and their subsequent use to elucidate the nature of the active site and the role of the various additives (bases and tri-methyl aluminium) in Ziegler-Natta catalysts.


Ziegler-Natta catalyst for polypropylene polymerization

In the early 1980s Brintzinger and Kaminsky demonstrated that homogeneous catalysts made up of Group 4 metallocenes could rival the traditional Ziegler-Natta catalysts in activity. Also, they are well defined and thus easy to modify. Since the 'metallocene revolution' the family of ac-


Prof. Tom Ziegler

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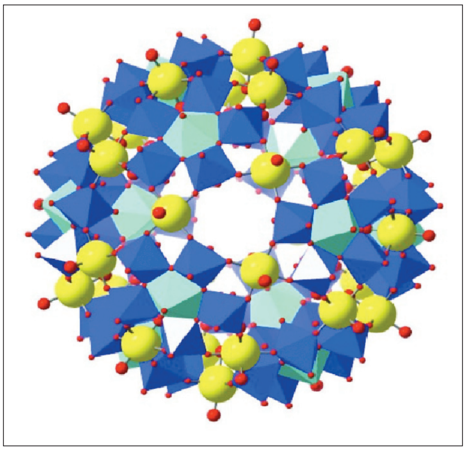
tive 'single-site' Group 4 complexes with or without Cp-ligands have grown considerably. Tom Ziegler demonstrated in the second part of his talk, how theoretical methods based on a combination of quantum mechanics and molecular mechanics can be used to understand the factors determining the activation of single-site catalysts, the rate of (polymer) growth and termination as well as catalyst decomposition and death.

In 1995 Maurice Brookhart demonstrated that complexes of late transition metals can also be used as single-site polymerization catalysts. The Brookhart catalysts are unique in that they can be used to control the morphology of the polymer by variations in T (temperature) and P (pressure) as well as the steric bulk around the metal. The Brookhart catalysts are in addition tolerant towards hetero-atoms such as oxygen and nitrogen, which makes it possible to use them in co-polymerization of ethylene with polar monomers such as acrylonitrile and methacrylate. The last part of the talk demonstrated how theoretical models can be used to simulate polymer growth as a function of T and P as well as the steric bulk around Brookhart catalysts. A discussion was also given on how computational methods can help in the design of catalysts that are able to co-polymerize olefins with polar monomers.

For further reading on this topic, please refer to [1].


Prof. Dante Gatteschi

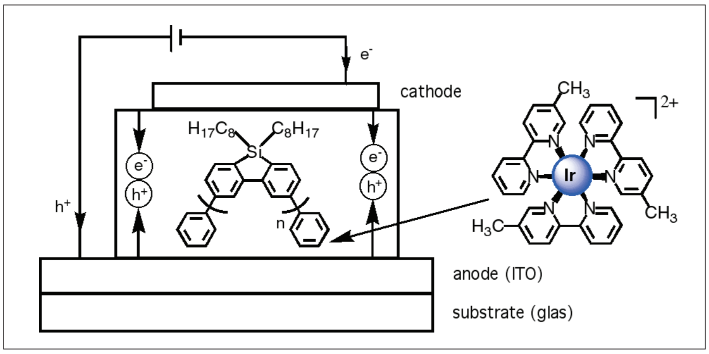
Dante Gatteschi (University of Florence) followed with his presentation on 'Molecular Nanomagnets'. His scientific activities are strongly affiliated to the European Network of Excellence (MAGMANET) which deals with all kinds of magnetic interactions. Molecular magnetism, in general, is a relatively new research area which involves the design, synthesis and characterization of new classes of magnetic materials that are based on molecules rather than metallic or ionic lattices of classical magnets. An exciting sub-area is that of molecular nanomagnets which encompasses large molecules, each containing a large number of interacting magnetic centres provided by metal ions, of both transition series and lanthanides, and/or organic radicals. Some molecules show slow relaxation of the magnetization at low temperature due to the concurring effects of a large spin in the ground state and a large magnetic anisotropy of the easy axis type. These molecules, in a sense, behave like tiny magnets, giving rise to magnetic hysteresis, and therefore, have been called single molecule magnets (SMM). The molecules are large and small at the same time and they have proved to be ideal candidates for studying quantum phenomena like tunnelling of the magnetization, in mesoscopic magnets. Apart from SMM, other types of molecular nanomagnets that are currently being investigated, are single chain magnets and antiferromagnetic rings.


The structure of [$Mo_{75}Fe_{30}$] clusters

For further reading on this topic, please refer the book recently published by the speaker [2].

The third lecture, entitled 'Design and Synthesis of Materials for Polymer LEDs', was given by ***Andrew B. Holmes*** (University of Melbourne). His group has synthesized the well-known emitting poly(*p*-phenylenevinylene) PPV material that has spiked interest in the development of new electrophosphorescent polymers. In his talk, he introduced the various attempts to prepare electrical conducting polymers by researchers such as Alan Heeger, Alan McDiarmid and Hideki Shirakawa which led to the Nobel Prize for that work in the year 2000. Polyfluorenes were the next interesting class of emitting polymers. The drawback of these compounds is the instability of the colour of emitted light. It changes


Prof. Andrew Holmes



LED with a suspended Ir-complex

slowly from blue to green. A certain stabilization was achieved by twisting the polyfluorenes, brought about by introducing a supplementary heteroatom in the central ring of the fluorene moiety. He explained the development of new host polymers based on poly(dialkyl-3,6-dibenzosilole) with high triplet energy (2.55 eV) for green electrophosphorescent emitters.

The nature of the applied emitters has a great influence on the colour of electrophosphorescence. Heteroleptic, *mer*-cyclometallated iridium complexes have been fine tuned from green to blue by changing the substituents on the pyridyl ring of the two phenylpyridyl ligands. As a third ligand, a trifluoromethane substituted pyridyltriazolyl ligand system was incorporated. Holmes's talk gave a deep insight into the difficulties encountered while constructing new light emitting compounds with well-adapted colours.

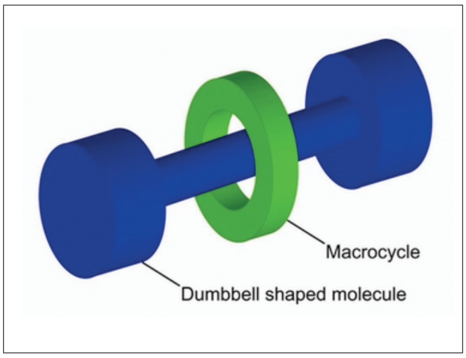
Further information about the work of Prof. Andrew Holmes can be found in the paper: 'Blue-to-green Electrophosphorescence of Iridium-based Cyclometallated Materials' [3].

J. Fraser Stoddart (UC Los Angeles) presented the last lecture of the day on 'Nano Meccano'. He is spearheading the field of molecular shuttles, catenanes, rotaxanes, molecular muscles and molecular machines. He started off his presentation with an explanation of the two terms 'nano' and 'meccano'. An overview of the existing molecular machinery like rotary motors, linear motors, molecular lifts and examples of hermaphroditic and palindromic molecular muscles were given. He elucidated that in such supramolecular assemblies, the units are not connected by conventional chemical bonds but by the so-called mechanical bonds. A well-established protocol for the construction of his very complex molecular devices was discussed which underscored the fact that it was only through the combination of all modern synthetic strategies that he was successful in building up those molecular machines. A careful control of the switching process between the two states of his machines was performed either by a photochemical or electrochemical process. A final excursion into the world of nanosensors showed the audience that molecular interactions between guest molecules and sensor molecules covalently attached to an AFM tip opens up a new world of applications which is still in its initial stages of development. The example of a chemically bonded dumbbell-shaped compound on a cantilever array of nanoscaled dimensions to mimic the movement of artificial muscles was an excellent piece of work. In the end, Stoddart initiated a very interesting discussion about the different ways to improve scientific skills and creativity. Stoddart's lecture has given a deep impression of the fact that we have not yet reached the end of the road with the conventional construction of covalently bounded molecules and that newer strategies combined with mechanically connected molecular units open an exciting field of supramolecular systems with novel and unexpected properties.

More details about the ingenious work of Prof. J. F. Stoddard can be found in 'Linear Artificial Molecular Muscles' [4].

In the closing remarks, Peter Belser emphasized the excellent quality of the four lectures. The success of the Spring Meeting 2006 was closely related to the generous financial support obtained from several industrial partners as well as the organizational support from the Division of Chemical Research of the Swiss Chemical Society.

Prof. J. Fraser Stoddart



Example of a [2]rotaxane molecule

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