NTNU

Norwegian University of
Science and Technology

The COREM Spring Meeting

May 12, 2017
Trondheim, Norway
G212 (EL2), Gamle Elektro
Elbygget, Etasje 2

Centre for Organic Electronic Materials (COREM)

COREM is a virtual centre which provides a scientific meeting place for people at NTNU and other Norwegian universities who research in the area of organic electronic materials such as solar cells, light emitting diodes (OLEDs), and field-effect transistors (OFETs). It originates from a collaboration between organic chemistry group and applied theoretical chemistry (ATC) group both located at the Department of Chemistry, NTNU. This collaboration has been generously funded by the Department who sees the research being conducted in organic solar cells as interesting and promising.

The research group

Bård Helge Hoff, Department of Chemistry, NTNU. Applied Organic Chemistry

Odd Reidar Gautun, Department of Chemistry, NTNU

Svein Sunde, Department of Materials Science and Engineering, NTNU.

John de Mello, Department of Chemistry, Imperial College London (UK)

Bjørn Kåre Alsberg, Department of Chemistry, NTNU. The Alsberg group

For more details, visit https://www.ntnu.edu/chemistry/research/corem

PROGRAMME
Friday, May 12, 2017

09:10 – 09:15	Welcome by Prof. Bjørn Alsberg
09:15 – 10:00	**Designing Multistep Organic Syntheses** *Assoc. Prof. Odd Reidar Gautun, Department of Chemistry*
Session Chair: Prof. Bjørn Alsberg	
10:00 – 10:30	**Dye Sensitized Solar Cells: Status and Outlook** *Dr. Vishwesh Venkatraman, Department of Chemistry*
10:30 – 10:45	*Coffee*
10:45 – 11:15	**Fabrication Process and Characterization of Dye-sensitized Solar Cells** *Audun Buene, Department of Chemistry*
11:15 – 11:30	**Phenothiazine-Graphene Hybrids for Dye-Sensitized Solar Cells** *Hugo Fougner, Department of Chemistry*
11:30 – 12:15	**Chemical stability of organic molecules and polymers used for light harvesting** *Prof. Bård Hoff, Department of Chemistry*
12:15 – 13:15	*Lunch*
Session Chair: Assoc. Prof. Odd Reidar Gautun	
13:15 – 14:00	**Chemometric optimization of organic synthesis** *Prof. Bjørn Alsberg, Department of Chemistry*
14:00 – 14:45	**Experimentally resolving polymeric structures from molecular to device scale** *Prof. Dag Breiby, Department of Physics*
14:45 – 15:00	*Coffee*
15:00 – 15:30	**Photochemistry - From Everyday Life to Energy Applications** *Dr. Solon Economopoulos, Department of Chemistry*
15:30 – 16:00	**Practical aspects of density functional theory** *Dr. Sailesh Abburu, Department of Chemistry*
16:00	Closing Comments

ABSTRACTS

Designing Multistep Organic Syntheses

Odd R. Gautun
Department of Chemistry, NTNU

How is it possible to plan and prepare complex molecules, which demand multistep synthesis in a logical and systematic manner? How do we choose the start materials?

The lecture will present some of the tools organic chemists may use for designing a practical synthetic scheme for a target molecule. The principles behind the concept of retrosynthetic analysis, also called the “disconnection” approach, by planning a synthesis backwards will be presented along with synthetic examples.

Dye Sensitized Solar Cells: Status and Outlook

Vishwesh Venkatraman
Department of Chemistry, NTNU

Dye sensitized solar cells (DSSCs) are of significant interest owing to their potential for low cost, large area, and/or flexible solar cells. This lecture provides an overview of the DSSC architecture with particular emphasis on the factors affecting the efficiency.

Fabrication Process and Characterization of Dye-sensitized Solar Cells

Audun Buene
Department of Chemistry, NTNU

For my talk I’ll be going through the fabrication process for DSSCs step by step. I’ll try to explain the reasoning behind each step and connect them to gains in cell performance, such as efficiency, stability and lifetime. I’ll include photos from our recent trip to the Grätzel/Hagfeldt lab at EPFL, and show you the current status for our own production process. Finally, some preliminary efficiency results for our own dyes will be presented.

Phenothiazine – Graphene Hybrids for Dye-Sensitized Solar Cells (DSSC)

Hugo Fougner,
Department of Chemistry, NTNU

Graphene-based materials have the potential to cater to a variety of nanotechnological applications ranging from optoelectronics, to biomedical as well as industrial. Can it be useful in DSSC?

The lecture will present an approach to synthesize dyes from phenothiazine and a way to attach them to graphene, as well as how to detect and characterize the graphene hybrids.

Chemical stability of organic molecules and polymers used for light harvest

Bård Helge Hoff
Department of Chemistry, NTNU

Alternative strategies for construction of solar cells and light emitting devices OLEDs are based on organic molecules/polymers as active material. Although the performance of the device is dependent on the materials morphological and mechanical stability, the chemical stability is the most important aspect as low stability directly leads to loss of performance and is likely to affect morphology and mechanical properties. The talk describes the major chemical stress factors and the typically reactions triggered leading to loss of conjugation and thus performance. Based on literature examples a few design guidelines for preparing stable molecules/polymers is presented.

Chemometric optimization of organic synthesis

Bjørn Kåre Alsberg
Department of Chemistry, NTNU

The current talk is tutorial introduction to the main ideas behind the use of experimental design and how it can be used in the optimization of organic synthesis. In particular there is a focus on the use of principal properties for selecting reagents, solvents, catalysts etc that improve on responses such as the yield, selectivity and cost. Experimental design is an important part of statistics and chemometrics where a minimum number of experiments are selected to extract the maximum amount of information. A core idea of the methodology is to discretisize the experimental space defined by a set of controllable factors. Discretization dramatically reduces the number of possible levels for each factor and thus the total number of experiments that can be performed. It is common to start an experimental design with only two levels for each factor: low (-) and high (+) whose corresponding true factor values are decided by the experimenter. Using this approach on factors such as the temperature and pH is straightforward, however it becomes more difficult when the factors are related to changes in the chemical structure. In this case it is better to use a new type of factor which is referred to as a principal property (PP) that can be obtained from performing principal component analysis (PCA) on a set of molecules. A PP is based on a linear combination of more fundamental properties. To compute PPs, PCA is applied to a dataset of molecules where each molecule is described by a set of descriptors that capture an aspect of their chemical structure such as proton NMR shifts, van der Waal volumes, dipole moments etc. It is then possible to perform experimental design in the PP space rather than the original space of structure descriptors. This allows us to search for combinations of solvents, catalysts etc that give us the best responses such as the yield or selectivity.

Experimentally resolving polymeric structures from molecular to device scale

Dag W. Breiby
Department of Physics, NTNU

Understanding the structure of polymers for organic electronics is a formidable task, not least because these materials exhibit a hierarchy of relevant length scales ranging from the molecular (~1 nm) to the device scale (~1 cm). For soft materials like polymers, the morphology can be tuned during the processing step through choice of solvent, shearing, and annealing, thereby giving access to a wide range of optical and mechanical

properties for each given material. An increasingly important scientific topic is to understand also the thermal properties of semiconducting polymers, which includes heat transfer, phase transitions, structural stability and thermoelectricity. In this talk, I will present experimental methods, mainly based on X-ray scattering and imaging, for addressing thin film morphologies. Our recent in situ studies of mesoporous films [1,2] and natural organic fibers exposed to humidity [3], micro-bead crushing [4], CO_2 accepting nanoparticles [5], thermoelectric thinfilms [6], and polymer thin film blends mounted on fast scanning calorimetry chips [7,8] will be highlighted.

[1] E.A. Chavez, H. Granlund, M. Sztucki, O. Konovalov, D.W. Breiby, A. Gibaud. ACS Appl. Mater. & Interf. 6 (2014) 2686-2691
[2] G.J.B. Voss, E.A. Chavez, A. Midttveit, J.B. Fløystad, K. Høydalsvik, A.Gibaud, D.W. Breiby, M. Rønning. J. Mater. Chem. A 2 (2014) 9727-9735
[3] M. Esmaeili, J.B. Fløystad, A. Diaz, K. Høydalsvik, M. Guizar-Sicairos, J.W. Andreasen, D.W. Breiby, Macromolecules 46 (2013) 434
[4] J.B. Fløystad, E.T.B. Skjønsfjell, M. Guizar-Sicairos, K. Høydalsvik, J. He, J.W. Andreasen, Z. Zhang, D.W. Breiby, Adv. Eng. Mater. 17 (2015) 545-553
[5] K. Høydalsvik, J.B. Fløystad, T. Zhao, M. Esmaeili, A. Diaz, J.W. Andreasen, R.H. Mathiesen, M. Rønning, D.W. Breiby, Appl. Phys. Lett. 104 (2014) 241909
[6] O. Bubnova, et al. Nature Materials 13 (2014) 190-194
[7] N. Patil, E.T.B. Skjønsfjell, N. Van den Brande, E.A. Chavez Panduro, R. Classens, M. Guizar-Sicairos, B. Van Mele, D.W. Breiby. PloS One 11 (2016) e0158345
[8] N. Van den Brande, N. Patil, M. Guizar-Sicairos, R. Claessens, G. Van Assche, D.W. Breiby, B. Van Mele. Organic electronics 41 (2016) 319-326

Photochemistry – From Everyday Life to Energy Applications

Solon Economopoulos
Department of Chemistry, NTNU

Photochemistry is a branch of science that surrounds many facets of our everyday life. We attempt to familiarize ourselves with photochemical processes that we encounter daily and move towards its importance when we deal with energy-related applications. Why is there a need to move away from fossil fuels towards more environmentally-friendly options? Can today's sustainable energy technology cover the increasing needs for electricity? Principles of third generation organic solar cells are presented alongside next generation materials like carbon nanotubes and we explore how energy-related applications can benefit from novel materials.

Practical aspects of density functional theory

Sailesh Abburu
Department of Chemistry, NTNU

Density functional theory (DFT) is the most commonly used technique to understand various chemical phenonmena and to estimate properties of molecules. Despite its popularity, the applicability of the method is limited due by the accuracy of property estimates. In this talk, I will present some of the practical aspects of using DFT - implementation using Gaussian 09 (for organic electronics applications), understanding the reasons for its limitations and ways to address them.