



Norwegian University of
Science and Technology

The first COREM Workshop

December 7-8, 2016
Trondheim, Norway
Realfagsbygget, R8

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
Wednesday, December 7, 2016

| | |
|---|---|
| 09:30 – 10:10 | Coffee |
| 10:10 – 10:20 | Welcome by <u>Head of Department, Dr. Marie-Laure Olivier,</u> <u>Department of Chemistry, NTNU</u> |
| <i>Session Chair: Prof. John de Mello</i> | |
| 10:20 – 11:10 | Crystal engineering for high-performance organic materials <u>Prof. John Anthony, University of Kentucky</u> |
| 11:10 – 11:30 | Coffee |
| 11:30 – 12:00 | Organic chemistry at NTNU: Towards organic electronic materials <u>Prof. Bård Hoff, NTNU</u> |
| 12:00 – 12:30 | Materials informatics for organic electronics <u>Prof. Bjørn K. Alsberg, NTNU</u> |
| 12:30 – 14:00 | Lunch |
| <i>Session Chair: Prof. Stelios Choulis</i> | |
| 14:00 - 14:50 | Synthesis of conjugated polymers for organic electronics. Making use of triplet excited states <u>Dr. Hugo Bronstein, University College London</u> |
| 14:50 – 15:20 | Water-soluble graphene-porphyrin trimers <u>Dr. Solon Oikonomopoulos, NTNU</u> |
| 15:20 – 15:40 | Coffee |
| 15:40 – 16:10 | Microfluidic routes to the controlled synthesis of electronic materials <u>Prof. John de Mello, Imperial College London</u> |
| 16:10 – 16:40 | Controlled synthesis of semiconducting polymers in droplet-flow microreactors <u>Dr. James Bannock, Imperial College London</u> |
| 16:40 – 16:45 | Closing Comments |
| 16:45 - 18:00 | Wine reception for speakers (Onsager room) |
| 19:00 | <i>Dinner: Restaurant Scandic Lerkendal</i> |

PROGRAMME
Thursday, December 8, 2016

| | |
|--|--|
| 09:00 – 10:00 | Tour of Nano Centre |
| <i>Session Chair Prof. John Anthony</i> | |
| 10:00 – 10:50 | The versatility of mesoscopic solar cells <u>Prof. Anders Hagfeldt, EPFL</u> |
| 10:50 – 11:20 | Synthesis of phenothiazine-based dyes for dye-sensitized solar cells <u>PhD student Audun Buene, NTNU</u> |
| 11:20 – 11:40 | <i>Coffee</i> |
| 11:40 – 12:30 | Materials and device engineering concepts for molecular and hybrid photovoltaics <u>Prof. Stelios Choulis, Cyprus University of Technology</u> |
| 12:30 – 14:00 | <i>Lunch</i> |
| <i>Session Chair: Prof. Bjørn K. Alsberg</i> | |
| 14:00 - 14:30 | Data-driven molecular design <u>Dr. Vishwesh Venkatraman, NTNU</u> |
| 14:30 – 15:00 | TBA <u>Prof. Per-Olof Åstrand, NTNU</u> |
| 15:00 – 15:20 | <i>Coffee</i> |
| 15:20 – 15:50 | Excitations in molecular systems <u>Dr. Espen Sagvolden, SINTEF/University of Oslo</u> |
| 15:50 – 15:55 | Closing Comments |

ABSTRACTS

Crystal engineering for high-performance organic materials

Prof. John Anthony

Department of Chemistry, University of Kentucky, USA

The electronic and photonic properties of organic materials in device-relevant configurations depends above all on the precise interactions between molecules in the solid-state. Materials for transistor applications, for example, require dense packing of molecules with precise interactions of the appropriate orbitals. For photovoltaics, these restrictions must be eased substantially to allow for proper heterojunction formation (while still allowing charge transport), and for singlet fission applications, these requirements are relaxed even further to prevent rapid recombination of photo-generated triplets. And for emissive devices, intermolecular electronic interactions must be eliminated entirely to prevent aggregation and fluorescence quenching. We have developed a robust functionalization scheme to control solid-state order in the acenes, an important class of organic electronic chromophore. Our exploration of the tuning of crystal structures has yielded high-performance hole-transporting materials for organic transistors, new non-fullerene acceptors for photovoltaics, benchmark singlet fission materials to enhance solar power generation, and compounds for tumor imaging using simple near-infrared radiation. The ability to generate high-quality X-ray crystallographic data on our compounds has allowed us to explore in detail the impacts of subtle defects on the performance of organic semiconductors, providing avenues for increased performance and efficiency. Until recently, all of this structural tuning has been highly Edisonian - chemical intuition suggesting synthetic targets, which must then be synthesized, tested, re-evaluated, and the process repeated. This approach requires preparation of dozens to scores of new compounds, with the parallel need of personnel time and hazardous waste generated by synthesis. We were recently awarded funds from the U.S. Materials Genome Initiative to explore computational methods to accelerate the materials discovery process. In particular, we are addressing computational prediction of crystal packing, the key parameter needed to understand the likely behavior of a material in device-relevant forms. To conclude my talk, I will present our results from the first portion of this research, which involves the development of a theoretical description of the interactions that influence solid-state order in silylethyne-substituted acenes.

Organic chemistry at NTNU: Towards organic electronic materials

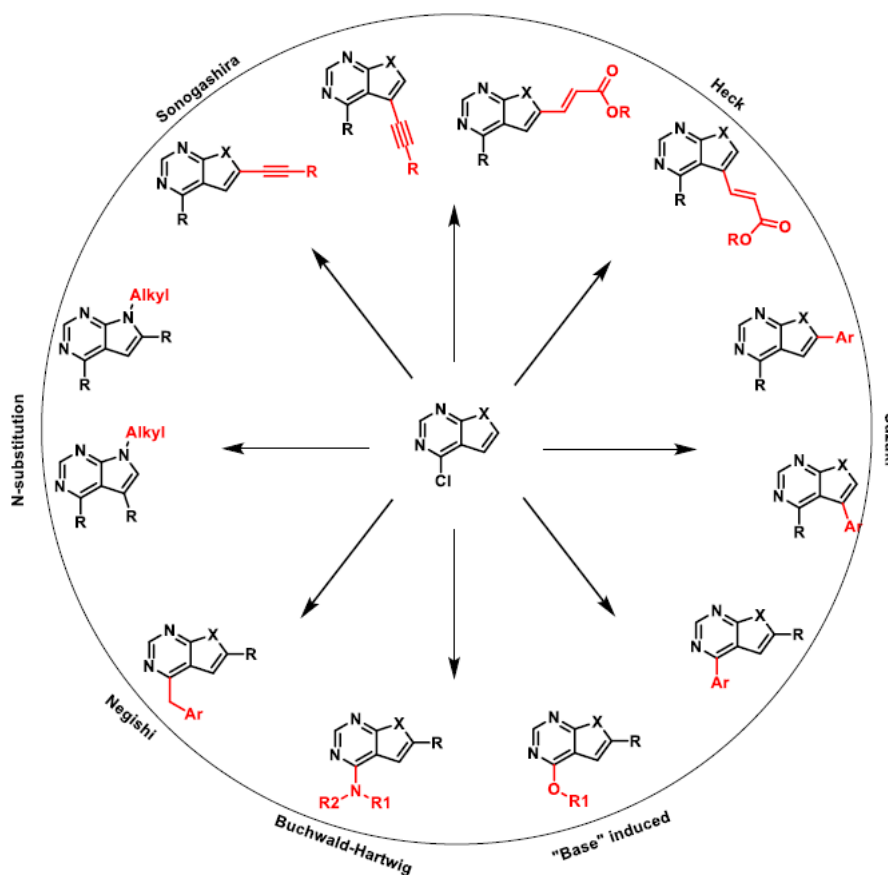
Prof. Bård Helge Hoff and Assoc. Prof. Odd Reidar Gautun

Department of Chemistry, Norwegian University of Science and Technology, Norway

Email: Bard.Helge.Hoff@chem.ntnu.no

A strategic change in research has been made in Section of Organic chemistry at NTNU. The newly focused research area is organic electronic materials. The lecture presents organic chemistry at NTNU, the competence of the two research groups involved in the work, our infrastructure, and

investments made to start build-up the new activity. An example will also be given on how we have worked on previous projects. We strongly believe that we are attractive partners within organic chemistry both on internal and external projects. Further, a new position in the field is expected to lead and boost future research.



Materials informatics for organic electronics

Prof. Bjørn K. Alsberg

Department of Chemistry, Norwegian University of Science and Technology, Norway

Email: bjorn.k.alsberg@ntnu.no

Typical research areas of interest for the field organic materials include organic solar cells, conductive polymers, organic light emitting diodes and organic field-effect transistors. A central challenge in the field is to make the discovery of new materials with improved properties more efficient and cost effective. An increasingly popular approach is to employ *materials informatics* where machine learning and computer science methods are used to facilitate the discovery and development of new materials. Here, our approach to materials informatics is presented which is based on *in silico* evolution of new molecules where structures are iteratively refined according to the principles of Darwinian evolution by optimizing one (or several) fitness value(s). These reflect the material property of interest such as conductivity, refractive index or power conversion efficiency. Our method is applied to different areas such as organic solar cells, in particular dye

sensitized solar cells (DSSC) also known as Grätzel cells, carbon capture (design of new amines and ionic liquids absorbents) and polymers (fine tuning of optical properties such as the refractive index). Central to our method is that the computation of the fitness value(s) need to be as efficient as possible since the evolutionary approach typically investigates thousands of structures to achieve significant fitness improvement. This limits the use of the most accurate quantum chemical (QC) methods such as density functional theory or coupled cluster. Thus another approach is employed where machine learning (ML) models replace computer intensive quantum chemical calculations. These models are often as accurate as QC methods, however suffer from being only locally valid which makes extrapolation risky. In this talk, an overview of the general method is presented with example applications.

Synthesis of conjugated polymers for organic electronics. Making use of triplet excited states

Dr. Hugo Bronstein

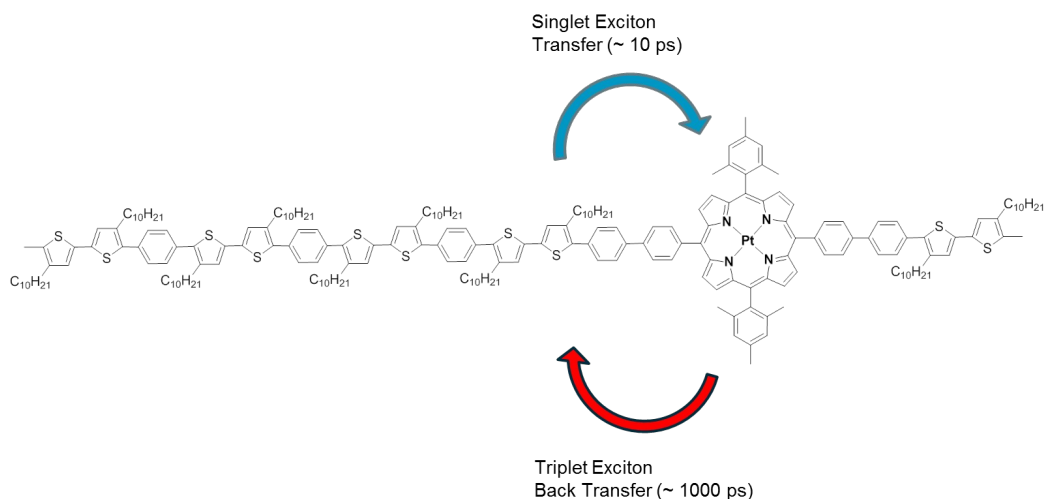
ERC Starting Grant Fellow and Lecturer
University College London, UK

Email: h.bronstein@ucl.ac.uk

Conjugated polymers are excellent candidates for use in next generation organic electronics due to their processability and tuneability. The excited state properties of these materials are relatively well explored with respect to their singlet states.

Triplet excited states, however, are both the cause and solution of many problems in the field of organic electronics. They affect the efficiency and stability of organic light emitting diodes and organic solar cells. Despite their immense importance within the field of organic optoelectronics and photochemistry in general, not much is known about their properties.

Here we present the synthesis and characterization of a conjugated polymers for use in organic solar cells and light emitting diodes where we can understand, manipulate and exploit the properties of the triplet excited state to overcome some of the fundamental limitations in these devices.



Water-soluble graphene-porphyrin trimers

Dr. Solon Economopoulos¹ and Prof. Nikos Tagmatarchis²

1 Department of Chemistry, Norwegian University of Science and Technology, Norway

2 National Hellenic Research Foundation, Theoretical and Physical Chemistry Institute, Greece

Email: solon.oikonomopoulos@ntnu.no

Graphene-based materials have the potential to cater to a variety of nanotechnological applications ranging from optoelectronics, to biomedical as well as, industrial. We present an efficient approach to anchor multichromophore systems, onto graphene through non-covalent interactions. The graphene itself has been prepared through ultrasonication processes, introducing minimal defects onto the graphitic backbone while affording comparatively large quantities that allow for chemical modification. The non-covalent attached graphene nanoensembles comprise of two different porphyrin systems, forming donor-donor-acceptor trimers. The porphyrin moieties are negatively and positively charged, respectively, and water soluble. Time-resolved photoluminescence experiments reveal the formation of an ultrafast component, attributed to the electronic communication of the electrostatically attached porphyrin with graphene offering improved electronic communication compared to p-p stacking.

All the synthesized products have been extensively characterized with microRAMAN, electrochemical and optical techniques (absorption, steady state and time-resolved photoluminescence spectroscopy) among others to verify, the structural and optoelectronic properties of the nanocomposites.

The introduction of these aqueous soluble materials opens up a wide array of artificial photosynthesis applications in electrochemical organic photovoltaic cells, while allowing more importantly for low-temperature deposition and precise optoelectronic chemical tailoring.

Microfluidic routes to the controlled synthesis of electronic materials

Prof. John de Mello

Faculty of Natural Sciences, Department of Chemistry, Imperial College London

Email: j.demello@imperial.ac.uk

Solution-based plastic electronics (PE) manufactured by fast roll-to-roll coating is an attractive technology for fabricating large-area electronic devices such as photovoltaic modules, lighting panels and displays at a fraction the cost of conventional electronics. However, for the technology to succeed, the cost and performance of PE materials and devices must be greatly improved relative to current levels. Here I will describe a new scalable approach to preparing high quality PE materials based on droplet microfluidics, which offers greatly improved control over materials

properties compared to conventional batch synthesis. The method can be applied to a broad range of electronic materials, including quantum dots, metal nanocrystals and semiconducting polymers, and offers a viable solution to the challenge of producing high quality PE materials in quantities sufficient for industrial application.

Controlled synthesis of semiconducting polymers in droplet-flow microreactors

Dr. James H. Bannock

Faculty of Natural Sciences, Department of Chemistry, Imperial College London

Email: j.bannock@imperial.ac.uk

Poly(3-hexylthiophene) (P3HT) is the mainstay semiconducting polymer for a broad range of organic electronic devices, and in particular thin-film organic photovoltaic (OPV) cells. Despite being over two decades since the first reported synthesis, there remains an unresolved problem with batch-to-batch consistency of P3HT in terms of electronic performance and solution rheology – both critical factors to the commercial success of printed OPV modules.

The primary cause of inconsistent electronic performance is the inability to source materials with consistent molecular weight distributions and purities. To address this obstacle we have developed a droplet-flow reactor approach for the preparation of P3HT, and other related conjugated polymers¹⁻³. In contrast to conventional flask methods which suffer from scaling issues above the few-gram level, our flow approach may be scaled up to production levels in excess of 1 kg/day without loss of control over the chemistry, and is sufficient to meet current industrial demand.

In this talk we will discuss the background concepts behind the droplet-flow approach, and we will demonstrate how these reactors may be used to prepare well-defined P3HT-based materials with predictable properties. We will show how our new variant of the polymerisation catalyst for P3HT provides a means of preparing polymers with a wide range of molecular weights while maintaining a high degree of control over the chain length polydispersity. We will further show how these droplet-flow reactors may be used to accurately tune the optoelectronic properties of P3HT by the controlled addition of an optically-distinct co-monomer into the polymer chain. To conclude we will discuss the use of bio-derived solvents in the P3HT synthesis, which enables full conversion to the product polymer to be achieved in just one minute - a significant reduction on flask methods that typically require several hours to reach completion.

(1) Bannock, J. H.; Krishnadasan, S. H.; Nightingale, A. M.; Yau, C. P.; Khaw, K.; Burkitt, D.; Halls, J. J. M.; Heeney, M.; de Mello, J. C. *Adv. Funct. Mater.* 2013, 23, 2123-2129.

(2) Bannock, J. H.; Al-Hashimi, M.; Krishnadasan, S. H.; Halls, J. J. M.; Heeney, M.; de Mello, J. C. *Mater. Horiz.* 2014, 1, 214-218.

(3) Bannock, J. H.; Xu, W.; Baïssas, T.; Heeney, M.; de Mello, J. C. *Eur. Polym. J.* 2016.

The versatility of mesoscopic solar cells

Prof. Anders Hagfeldt

Laboratory of Photomolecular Science, Swiss Federal Institute of Technology Lausanne (EPFL),
CH-1015, Lausanne, Switzerland

Email: Anders.Hagfeldt@epfl.ch

In our work on solid-state dye-sensitized solar cells (ssDSSC) we have recently [1] shown that copper phenanthroline complexes can act as an efficient hole transporting material. We prepared ssDSCs with the organic dye LEG4 and copper(I/II)-phenanthroline as redox system and achieved power conversion efficiencies of more than 10%. Our follow up work on electron transfer studies and device optimization will be presented at the meeting.

In our work on perovskite solar cells (PSC) we have achieved efficiencies above 20% with a mixed composition of iodide/bromide and methyl ammonium/formamidinium [2]. For cells larger than 1 cm² we recently certified a record efficiency of 19.6% [3], replacing the anti-solvent step in the perovskite film formation with a vacuum flash treatment. With the use of SnO₂ compact underlayers as electron acceptor contacts we have constructed planar perovskite solar cells with a hysteresis free efficiency above 20% [4]. Recently, we have taken the cation mixing of the perovskite film further by including the Cs⁺ in a so-called 'triple cation' composition, i.e. Cs/FA/Ma. Larger grains grown in a monolithic manner are observed and for example reproducibility and device stability are improved [5]. At the meeting we will discuss our follow up works and present our champion data; up to 22% efficiency with an external electroluminescence of 4%, and an outstanding open-circuit voltage of 1.24 V at a band gap of 1.63 eV entailing one of the smallest loss-in-potential of 0.39 V ever measured for any solar cell material [6]. Furthermore, we will report a breakthrough in stability at 85 °C for 500 h under full solar illumination and maximum power point tracking (during which 95% of the initial performance was retained).

References

- [1] Freitag et al., Energy & Envir. Sci., DOI: 10.1039/C5EE1204J
- [2] Bi et al., Science Advance, DOI: 10.1126/sciadv.1501170
- [3] X. Li et al., Science, DOI:10.1126/science.aaf8060
- [4] Correa et al., Energy & Envir. Sci., DOI:10.1039/C5EE02608C
- [5] M. Saliba et al., Energy & Envir. Sci., 2016, DOI: 10.1039/C5EE03874J
- [6] M. Saliba et al., Science, 10.1126/science.aah5557 (2016)

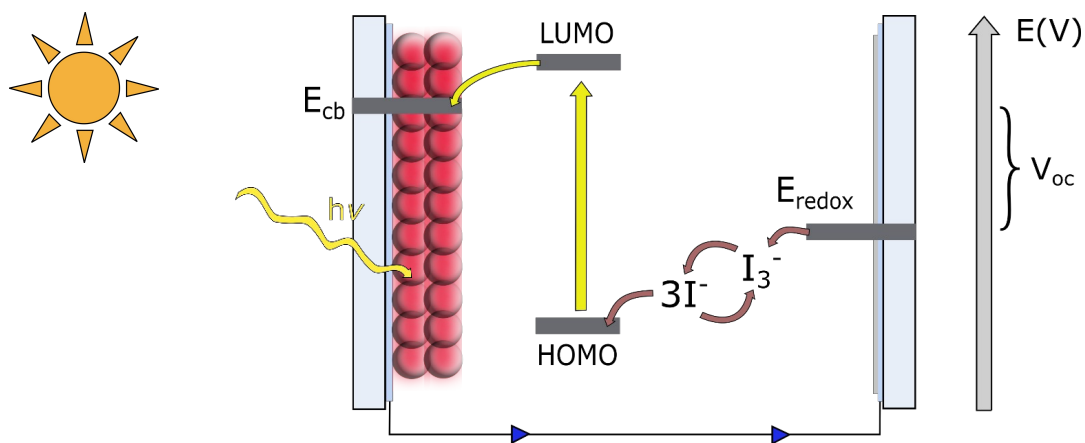
Synthesis of phenothiazine-based dyes for dye-sensitized solar cells

Audun Formo Buene and Prof. Bård Helge Hoff

Department of Chemistry, Norwegian University of Science and Technology, Norway

Email: audun.f.buene@ntnu.no

Dye-Sensitized Solar Cells (DSSCs) are promising candidates to replace or complement the traditional silicon-based solar cells of today. The introduction of organic solar cells may reduce the production cost of solar energy and additionally enable energy production from applications in environments where this was previously unthinkable, such as low/diffuse light or indoor applications.



Our group in Trondheim has focused on developing new dye molecules for DSSCs, and evaluating their behavior. Understanding how the properties of the dyes can be tuned to achieve certain properties is of great interest. Molecular properties of particular interest are absorption wavelength, extinction coefficient, stability, non-crystallinity and ultimately the photon-to-electron conversion efficiency (PCE).

The focus of this talk is the development of synthetic routes allowing access to a large variety of dye molecules, thus making it possible to investigate several structure related properties. Over 20 new dyes have been synthesized via the established synthetic routes so far, and are currently under evaluation.

Materials and device engineering concepts for molecular and hybrid photovoltaics

Prof. Stelios A. Choulis

Molecular Electronics and Photonics Research Unit, Department of Mechanical Engineering and Materials Science and Engineering, Cyprus University of Technology, Cyprus

Email: stelios.choulis@cut.ac.cy

The advantages of Solution Processed molecular and hybrid Photovoltaics, such as their light weight, mechanical flexibility in addition to the small energy demand, and low cost equipment requirements for roll-to-roll printing mass production, characterize them as a dominant candidate source for future electrical power¹. The Presentation aims in covering a range of engineering and underpinning scientific issues needed to bring printed (organic and perovskite) solar cells^{2,3} to commercial viability in terms of efficiency⁴, lifetime⁵ and cost⁶. A systematic understanding of the

relationship between materials structure, processing, properties and device performance relevant to printed photovoltaics product development targets will be presented.

ACKNOWLEDGEMENTS: Funding from the *ERC* (H2020-ERC-2014-GoG project number 647311) and PLASMAS SME based EU-Project No. 604568 are gratefully acknowledged.

[1] Hoth, C.N., Schilinsky, P., Choulis, S.A., Brabec, C.J., *Nano Letters* 2008, Vol. 8 (9), pp. 2806-2813.

[2] Wenchao Zhao, Deping Qian, Shaoqing Zhang, Sunsun Li, Olle Inganäs, Feng Gao, Jianhui Hou, *Advanced Materials*, 2016; **DOI:** 10.1002/adma.201600281

[3] Saliba M, Matsui T, Seo J-Y, Domanski K, Correa-Baena J-P, Nazeeruddin MK, Zakeeruddin SM, Tress W, Abate A, Hagfeldt A, Grätzel M. *Energy and Environmental Science*, **2016**. **DOI:** 10.1039/C5EE03874J

[4] Burgués-Ceballos, I., Hermerschmidt, F., Akkuratov, A. V., Susarova, D. K., Troshin, P. A., Choulis, S. A., *ChemSusChem*, 2015, DOI: 10.1002/cssc.201501128

[5] Savva, A., Burgués-Ceballos, I., Choulis, S.A. *Advanced Energy Materials*, 2016, DOI: 10.1002/aenm.201600285

[6] Neophytou, M., Georgiou, E., Fyrrillas, M.M., Choulis, S.A., *Solar Energy Materials and Solar Cells* 2014, Vol. 122, pp. 1-7

Data-driven molecular design

Dr. Vishwesh Venkatraman

Department of Chemistry, Norwegian University of Science and Technology, Norway

Email: vishwesh.venkatraman@ntnu.no

Given the huge combinatorial space of chemical structures, searching for new materials with tailored properties is a very difficult task. In recent years, there has been a significant thrust towards the use of mathematical frameworks for molecular design via statistical learning. These informatics aided approaches can dramatically shorten the time and effort needed to discover and develop new materials, but are faced with the problem of sparse amount of reliable experimental and related computationally derived results. Also, when using such mathematical tools to model structure-property relationships, it becomes necessary to gauge the reliability of predictions made for instances outside the training pool. This presentation examines the issues and challenges in applying data-driven approaches to molecular discovery, in particular to dyes for dye-sensitized solar cells.

TBA

Prof. Per-Olof Åstrand

Department of Chemistry, Norwegian University of Science and Technology, Norway

Email: per-olof.aastrand@ntnu.no

Excitations in molecular systems

Dr. Espen Sagvolden

University of Oslo/SINTEF, Norway

Email: espen.sagvolden@kjemi.uio.no

Excitations, their ability to survive, diffuse and cause charge-separation are central in organic photovoltaics. I will discuss how excitations are computed in quantum chemistry and some pitfalls of such computations. By drawing on computations on the excited states of the 2-pyridone dimer, I discuss the tug of war between those forces causing localization and delocalization of excitations in molecular crystals. Finally, the mechanisms of excitation energy transfer are discussed.
