



European Photochemistry Association

NEWSLETTER

December 2007

General information about the European Photochemistry Association

is available at:

www.photochemistry.eu

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EDITORIAL

Chair's Letter

Dear Colleagues,

At the last General Assembly of EPA in Cologne (page 6), I succeeded David Phillips whom I would like to thank warmly for his contribution to the Association. In his Chairman's Letter one year ago, David Phillips remarked that *"the EPA has been declining in membership and activity over the past decade or so, as the subject of Photochemistry has become more fragmented"*. All the members of the Executive Committee agreed with that statement and decided to make serious efforts to revive our Association. Even when working at the interface with other disciplines (atmospheric chemistry, nanosciences, material sciences, photobiology, medicine....) correct understanding of the fundamental principles which govern the interaction between light and molecular systems remains crucial. In this respect, systematic contacts among photochemists guarantee a better quality in our work. Furthermore, the existence of EPA constitutes recognition of this discipline both among the scientific community and in the civil society.

Keeping EPA vibrant and capable of attracting young scientists can be achieved only by taking into account the current European and international context which has changed greatly since the creation of our Association in 1970. The Executive Committee has undertaken a series of actions towards this direction, each one of the members having a particular task to achieve (page 9).

To start with, we wish to facilitate membership renewal and application by introducing a centralised easy-to-use credit card payment system (page 69). It is already possible to use this simplified procedure for 2008 membership fees. I would like to take this opportunity to highlight the benefits of being an EPA member. First of all, EPA members have electronic access to Photochemical & Photobiological Sciences, the official Journal of the Association (page 13). In addition, members will benefit from reduced registration fees, for example, for the forthcoming IUPAC Symposium on Photochemistry to be held in Gothenburg, Sweden (page 59). Two important events will take place at the Gothenburg Symposium which members are encouraged to attend: the Executive Committee will propose a revision of the statutes to the EPA General Assembly and the first PhD prize in Photochemistry will be awarded with the laureate presenting his/her work.

You are invited to visit our new website (www.photochemistry.eu) which will have a member-only area shortly, with a lively discussion forum. Exchange of information among members is also encouraged through an e-mailing list.

As many of you have requested, from 2008 a printed version of the Newsletter will be distributed to members. I look forward to announcing further exciting developments in the next issue of the Newsletter.

Dimitra Markovitsi
EPA Chair

MINUTES OF THE EPA GENERAL ASSEMBLY

Place: Department of Chemistry of the University of Cologne, Kurt-Alder Lecture Hall, July 30th 2007, 19.00 to 20.00 h. Attendance: 42 members and one non-member from 18 countries

Agenda:

1. Welcome by Chair
2. Review of current statutes
3. Chairman's report
4. Treasurer's reports 2004-2006
5. PPS issues
 - 5.1 Report by Sarah Ruthven, RSC
 - 5.2 EPA membership fee/PPS subscription
6. Decision on EPA membership fee 2007
7. Rules for EPA Prize for PhD Thesis
8. Nominations for Chair
9. Election of new members of Executive Committee
10. Any other business

1. The Assembly was opened by Chair David Phillips. The Agenda for the present assembly were adopted.
2. Chair David Phillips made a survey of the current statutes of EPA: EPA has three Organs, General Council (GC), Standing Committee (SC), and Executive Committee (EC), all with different tasks. He stated, that only two organs, CC and EC, exist in practice, and in many respects, e.g. in election of the EC, the statutes cannot be obeyed. Chair repeated the opinion of the current EC, that the statutes of EPA should be changed in future to satisfy the changed situation and practice.
3. Chair David Phillips reported about the activity of the EC for the last three years.
 - Executive committee has met once per year [2006/2007]
 - On-line Newsletter has been revived, thanks to Dimitra Markovitsi
 - Web-site revived, due to Eric Vauthey
 - Chair and Sandra Monti represented EPA on several meetings of Ownership Board of PPS
 - Despite the efforts by Chair and Treasurer, Membership lists are still unsatisfactory; according to Sarah Ruthven, RSC could help in this respect. Better dialogue with national organisations is needed.
 - Plan to offer EPA prize for best PhD thesis agreed, to be implemented at IUPAC Symposium, 2008
4. The financial statements provided by the Treasurer, Silvio Canonica, for the years 2004 - 2006 were presented.
5. PPS issues
 - 4.1 Report by Sarah Ruthven.
PPS Editor Sarah Ruthven, RSC, made a survey of the current quality of PPS, demonstrating by several parameters, that the respect of the journal has increased substantially.
 - 4.2 EPA membership fee/PPS subscription

Chair David Phillips considered the relation of PPS to EPA by stating the facts that

- [1] PPS is part-owned by EPA
- [2] PPS is published by RSC
- [3] PPS is successful, has highest impact factor of all photo-chemical/biological journals.
- [4] At present, cost of PPS subscription exceeds EPA membership fee, thus EPA finances are declining.
- [5] RSC has offered partial solution. For those EPA members whose institution has taken out an institutional subscription, on-line access to PPS will be offered free to individual members.
- [6] Issue needs to be resolved, either by increase in EPA fee, or change to PPS subscription arrangement. The changes must be discussed before implementation at PPS Ownership Board in Bath, September 2007; earliest implementation, January 2009

6. Decision on EPA membership fee 2008

The EC proposed for the 2008 EPA membership fee the following

- The fees will be paid in Euros
- Full membership 30 Euros per annum
- Student membership, i.e. PhD students, 15 Euros per annum
- East Europe, non-EU countries, concession 15 Euros per annum
- Concession for retired members to be abolished

The proposal was adopted unanimously.

7. Rules for the EPA Prize for PhD Thesis

- The EC proposed the following Rules for the EOA PhD Prize:
- Prize is offered every two years, with presentation at IUPAC symposium
- Prize is 1000 Euros, plus travel costs to IUPAC symposium (for a maximum of 300 €), one free year of EPA membership
- Students to be nominated by EPA member
- The nomination should include a copy of the thesis; an abstract of thesis in English, no more than five pages; a list of publications arising from the thesis; a letter of support
- Ad hoc judging committee to be nominated by Executive Committee

The proposal was adopted unanimously.

First competition for all theses awarded Ph.D in 2006/2007
Decision early in 2008

8. Nominations and election for Chair

The Executive Committee had asked the Local Treasurers of EPA, in spring 2007 and for the last time on 29th of June 2007, EPA to circulate National EPA members seeking nominations for a new EPA Chairperson to replace David Phillips, who is retiring as EPA Chairman in August 2007. Only one nomination has been received: Dimitra Markovitsi, CNRS Research Director and Head of the Francis Perrin Laboratory, France (<http://www.lfp.cea.fr/>). She is a Member of the EPA Executive Committee and Editor of the EPA Newsletter. Her research interests are focused on the interaction of UV radiation with DNA, collective effects in organized molecular systems and time-resolved spectroscopy. She has two European Nationalities, French and Greek.

Dimitra Markovitsi was elected unanimously to the chair for August 2007 - July 2008.

9. Election of new members of Executive Committee

The Executive Committee for the period 2004-2007

- David Phillips [UK], chair
- Helge Lemmetyinen, [Finland]
- Silvio Canonica [Switzerland]
- Sandra Monti [Italy]
- Eric Vauthey [Switzerland]
- Dimitra Markovitsi [France]
- Nina Gritsan [Russia]

was re-elected unanimously for the next period, with the change of chair as decided in the previous paragraph and with the addition that David Phillips stayed as a member of EC.

In addition the EC was complemented by

David Worrall [UK],

Werner Nau [Germany], and

one seat was reserved to be nominated by the Spanish EPA community.

10. Any other business

There was none.

11. The assembly was closed at 20.00 by the chair.

August 7th, 2007

Helge Lemmetyinen
Secretary of the Assembly

EPA EXECUTIVE COMMITTEE



Chair

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EPA PhD PRIZE

EPA prize for PhD Thesis on Photochemistry

The first EPA Prize will be attributed during the XXIIInd IUPAC Symposium on Photochemistry which will be held in Gothenburg, Sweden, from July 28 – August 1, 2008. The awarded will present their work at the Symposium.

The Prize is 1000 Euros, plus travel costs to Gothenburg (within the limit of 300 €) and one free year of EPA membership.

The candidate must:

- have defended his PhD Thesis in 2006/2007
- be nominated by an EPA member

Deadline for nominations: end of 2007

Please send nominations, including

- [1] a copy of the thesis
- [2] an abstract of thesis in English, no more than five pages
- [3] a list of publications arising from the thesis
- [4] a letter of support,

to the EPA Chair:

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E-mail: dimitra.markovitsi@cea.fr

PHOTOCHEMICAL AND PHOTOBIOLOGICAL SCIENCES

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 - IUPAC Gold Book terms linked

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Rex Tyrrell,
Bath, UK



Frans De Schryver,
Leuven, Belgium

Parameters affecting the chemical work output of a hybrid photoelectrochemical biofuel cell

Michael Hambourger, *et al.*, USA *Photochem. Photobiol. Sci.*, 2007, **6**, 431

Highly efficient supramolecular photocatalysts for CO₂ reduction using visible light

Shunsuke Sato, *et al.*, Japan *Photochem. Photobiol. Sci.*, 2007, **6**, 454

Conformational analysis of the blue-light sensing protein YtvA reveals a competitive interface for LOV-LOV dimerization and interdomain interactions

Valentina Buttani, *et al.*, Italy *Photochem. Photobiol. Sci.*, 2007, **6**, 41

Intracellular photodynamic therapy with photosensitizer-nanoparticle conjugates: cancer therapy using a Trojan horse

Martina E. Wieder, *et al.*, UK *Photochem. Photobiol. Sci.*, 2006, **5**, 727

Synthesis, structure and luminescence studies of heterometallic gold(I)–copper(I) and –silver(I) alkynyl clusters/aggregates

Sung-Kong Yip, *et al.*, China *Photochem. Photobiol. Sci.*, 2007, **6**, 365

Relation between intracellular location and photodynamic efficacy of 5-aminolevulinic acid-induced protoporphyrin IX *in vitro*. Comparison between human glioblastoma cells and other cancer cell lines

Reinhard Sailer, *et al.*, Germany *Photochem. Photobiol. Sci.*, 2007, **6**, 145



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ACTIVITIES OF NATIONAL GROUPS: UNITED KINGDOM

Activities of the UK Photochemistry community

During the latter half of 2007, I wrote to individuals in all UK universities who I had identified as having research activity in photochemistry, photophysics or photocatalysis, asking for research highlights from their groups and universities. Below are the reports from those groups able to respond in time for publication in this newsletter. Hence the activity described below is not comprehensive, but I hope provides a flavour of the diverse and vigorous UK photochemistry community.

Dr. David Worrall, Loughborough University

Cardiff University

The group has fifteen years experience in photocatalysis and focuses exclusively on anaerobic photocatalysis for the production of hydrogen. This includes water splitting and the reforming of simple hydrocarbons such as methanol and ethanol. The process involves the synthesis of metal-titania photocatalysts (note that, unlike for oxidative photocatalysis, *titania alone is near-useless in anaerobic conditions*). For methanol-water reforming using light, three moles of hydrogen are produced for each methanol consumed, since one mole of water is also consumed. The mechanism of the reaction involves dehydrogenation of the organic on the metal component, photo-excitation of states within the titania which produces a highly reactive oxidant ($O^{\cdot-}$) which in turn oxidises otherwise blocking fragments (such as CO) on the metal component, thus ensuring steady-state turnover. The threshold for the reactions is the bandgap of titania, and, like other groups in the world, we are currently engaged in modifying the titania to encompass longer wavelengths of sunlight. We are also currently researching the use of gold for such reactions.

Professor Michael Bowker
Wolfson Nanoscience Laboratory
School of Chemistry
Cardiff University

University of East Anglia

Researchers at the University of East Anglia are investigating the photophysics of the green fluorescent protein chromophore and the excited state dynamics of intact GFP using ultrafast spectroscopy. In the former they worked out the mechanism of the surprisingly efficient radiationless decay. This led them to some conclusions on how the protein suppresses the relaxation. They also studied the ultrafast motion along a proton wire which dominates the photophysics of the intact GFP, using femtoseconds IR and mutagenesis.

K. Litvinenko, N. M. Webber and S. R. Meech, 'Internal Conversion in the Chromophore of the Green Fluorescent Protein: A Temperature and Isoviscosity Analysis' J. Phys. Chem. A, 2003, 107, 2616 - 2623.

D. Mandal, T. Tahara and S. R. Meech 'Excited State Dynamics of The Green Fluorescent Protein Chromophore' J. Phys. Chem. B 2004, 108, 1102 - 1108.

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D. Stoner-Ma, A. A. Jaye, P. Matousek, M. Towrie, S. R. Meech and P. J. Tonge 'Observation of Excited State Proton Transfer in Green Fluorescent Protein Using Ultrafast Vibrational Spectroscopy' J. Amer.Chem. Soc. (Communication), 2005, 127, 2864 - 2865.

A. A. Jaye, D. Stoner-Ma, P. Matousek, M. Towrie, P. J. Tonge and S. R. Meech, 'Time Resolved Emission Spectra of the Green Fluorescent Protein (GFP)' Photochem-Photobiol (GFP symposium in print) 2006, 82, 373 - 379.

D. Stoner-Ma, E. H. Melief, J. Nappa, K. L. Ronayne, M. Towrie, P. J. Tonge and S. R. Meech 'Proton Relay Reaction in Green Fluorescent Protein (GFP): Polarization Resolved Ultrafast Vibrational Spectroscopy of Isotopically Edited GFP' J. Phys. Chem. B 2006, 110. 22009 - 18

They also employ steady state and dynamic experiments to investigate photoprocesses at the surface, in particular hot electron attachment to adsorbates at metal surfaces and photoemission from ice surfaces. They observed a novel surface plasmon enhancement on silver metal and an extremely low photoemission threshold for Na doped ice.

T. Vondrak, D. J. Burke and S. R. Meech, 'The Dynamics and Origin of NO Photodesorbed From NO/Ag(111)' Chem. Phys. Lett., 2000, 327, 137 - 142.

R. T. Kidd, D. Lennon and S. R. Meech, 'Surface Plasmon Enhanced Substrate Mediated Photochemistry on Roughened Silver' J. Chem. Phys., 2000, 113, 8276 - 8282.

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D. J. Burke, T. Vondrak and S. R. Meech 'Photochemistry Of Fe(CO)₅ Adsorbed On Single Crystal and Roughened Silver' J. Phys. Chem. B, 2002, 106, 10205 - 10214.

D. J. Burke, T. Vondrak and S. R. Meech 'Photodesorption And Photochemical Dynamics On Roughened Silver: Sulphur Dioxide And Carbonyl Sulphide' Surface Science, 2005, 585, 123 - 133.

T. Vondrak, J. M. C. Plane and S. R. Meech 'Two-Photon Photoemission from the Cu(111)-Ice Surface' J. Phys. Chem. B (Letter), 2006, 110, 3860 - 3.

Stephen Meech
School of Chemical Sciences and Pharmacy
University of East Anglia

The University of Edinburgh

We have developed a new experimental approach to the study of photochemical reactions, in which laser radiation is coupled into the probe of an NMR spectrometer, enabling the NMR spectra of transient photoproducts to be obtained. Use of this technique in combination with *ab initio* quantum chemical calculations has revealed the previously inaccessible structures of the elusive *cis* isomers of azo dyes.^{1,2} We have pioneered the use of time-resolved spectroscopy of the fluorescent adenine analogue, 2-aminopurine, to study the conformational behaviour of DNA.³ The application of this technique, in combination with x-ray crystallography, to single crystals of DNA-enzyme complexes is proving particularly powerful in elucidating the mechanism of reactions in which DNA bases are chemically modified.^{4,5} We have developed fluorescence lifetime imaging microscopy (FLIM) as a tool for quantitative spatial mapping of physical measurands, such as fluid composition (mixing) and temperature in microfluidic devices.⁶ The quantitative data obtained from FLIM are being used to validate computational models of diffusion and heat transfer on the microscale, with a view to the development of *a priori* methods for the design of microfluidic devices.

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2. Structural characterisation of the photoisomers of reactive sulfonated azo dyes by NMR spectroscopy and DFT calculations, Katrina M. Tait, John A. Parkinson, David I. Gibson, Patricia R. Richardson, Warren J. Ebenezer, Michael G. Hutchings and Anita C. Jones, *Photochem. Photobiol. Sci* (in press; published on web 20 April 2007)
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4. Time-resolved fluorescence of 2-aminopurine as a probe of base flipping in M.HhaI-DNA complexes. Neely, Robert K.; Dajotyte, Dalia; Grazulis, Saulius; Magennis, Steven W.; Dryden, David T. F.; Klimasauskas, Saulius; Jones, Anita C., *Nucleic Acids Research* 2005, 33, 6953-6960.
5. 2-Aminopurine flipped into the active site of the adenine-specific DNA methyltransferase M.TaqI: crystal structures and time-resolved fluorescence, Thomas Lenz, Eleanor Y. M. Bonnist, Goran Pljevaljčić, Robert K. Neely, David T. F. Dryden, Axel J. Scheidig, Anita C. Jones and Elmar Weinhold, *J. Am. Chem. Soc* 2007, 129, 6240-6248.
6. Quantitative spatial mapping of mixing in microfluidic systems. Steven W. Magennis, Emmelyn M. Graham, Anita C. Jones, *Angew. Chem. Int. Ed.* 2005, 44, 6512-6516.

Dr. Anita C. Jones
School of Chemistry
The University of Edinburgh

University of Glamorgan

Our interests are in the photochemistry and photophysics of molecules which can act as fluorescent probes and sensors. We are interested in their absorption and emission properties in different media; this encompasses both spectral and kinetic measurements at timescales down to fs. The classes of compounds that we are working with include 4-*N*-alkylamino-1,8-naphthalimides, TICT compounds related to DMABN and dyes which undergo excited state intramolecular proton transfer based on the 3-hydroxyflavone and 2-(2'-hydroxyphenyl)benzazole systems.

We are also undertaking studies of photochromic materials (particularly of naphthopyrans) with particular emphasis on modelling the slow (seconds to minutes) kinetics.

Bob Brown
Faculty of Health, Sport & Science
University of Glamorgan

University of Glasgow

In an EPSRC funded Discipline Hopping Grant collaboration involving Dr Andy Burrows (Department of Chemistry, University of Bath) and Dr Markus Kraft (Department of Chemical Engineering, University of Cambridge), Dr Justin Hargreaves (Department of Chemistry, University of Glasgow) is investigating the influence of preparative routes on the photocatalytic activity of titania. This project centres upon the controlled modification of titania systems, by eg nitrogen doping, with the aim of producing visible light active materials which are well-defined both in terms of TiO₂ morphology/composition and size distribution and the chemical form of dopant. By inter-relating such parameters with activity measurements, it is hoped to further elucidate the origin of catalytic activity with the aim of gaining enhanced understanding of the origin of photocatalytic activity and the further improvement of activity. Particular emphasis is being placed upon the preparation of catalysts by flame synthesis involving organometallic precursors containing dopant elements and post-synthetic modification by procedures such as ammonolysis.

Dr Justin Hargreaves
Department of Chemistry
University of Glasgow

Glasgow Caledonian University

At Glasgow Caledonian university there is a long standing interest in the acute and chronic effects of ultraviolet radiation (UVR) on the eye, whether this be related to safety in the workplace (e.g. welders) or changes in our environment. The main ongoing research interests are on the cornea and conjunctiva in relation to UVR.

Michael J. Doughty, PhD
Glasgow-Caledonian University
Department of Vision Sciences

Lancaster University

Analytical chemists at Lancaster University investigating the environment fate of pesticides and other trace persistent organic pollutants in the environment. They have a long-running interest in the environmental fate of these chemicals, particularly their atmospheric transport and accumulation in cold environments like the Arctic.

Recent funding from NERC and from one of the Agrichem companies has allowed the investigation of photochemical degradation/behaviour of two structurally similar organophosphorus pesticides in snow/ice and enabled comparison to "standard" aqueous degradation tests. This work was conducted in conjunction with a team at Masaryk University in the Czech Republic who specialise in chemical degradation experiments at sub-zero temperatures. So far they have found that the degradation rates in ice are much slower compared to those in water, and that competing hydrolytic processes are effectively 'switched off' in ice, resulting in several intermediates being present in ice for much longer periods than they are in water. As these photodegradates are of more toxicological concern than the parent compounds, then this could have environmental implications following their release with the onset of seasonal snow-melt.

This work is part of a 'degradation and fate' laboratory, which has photochemical tests as a central component, and has been set up as part of the Centre for Chemicals Management. (<http://www.lec.lancs.ac.uk/ccm/research/degradation/index.htm>)

Dr C. J. Halsall
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The photochemistry research group at Loughborough is currently investigating electron-transfer and energy-transfer on insulator surfaces, these studies involving collaboration with the Ukrainian Academy of Sciences (Kiev) and the Association for the Cultivation of Science (Calcutta, India). The photochemistry and photophysics of singlet oxygen in supercritical fluids (CO₂ and xenon) are the basis of an international collaboration with Ain Shams University (Cairo, Egypt).

Nanosecond time resolved diffuse reflectance laser flash photolysis is being used to study a variety of uni- and bimolecular processes on the surfaces of both silica gel and microcrystalline cellulose. The processes studied include triplet-triplet annihilation, triplet-triplet energy transfer and electron transfer between cation radicals of anthracene and a number of electron donors. Kinetic models are also being developed to describe these processes in terms of fractal- and two-dimensional rate constants, and also in terms of a dispersive kinetic model assuming a distribution of rate coefficients. Monte-Carlo simulations are used to correlate fitted parameters with physical models of the behaviour of molecules on surfaces.

Triplet-triplet energy transfer and photoinduced electron transfer are being used to study diffusional characteristics and clustering effects in modified supercritical fluid carbon dioxide. Supercritical fluid Xenon is being investigated as a medium in which to study excited triplet state reactions since we have demonstrated that intersystem crossing yields are significantly enhanced in this fluid relative to organic solvents. The generation and subsequent fate of singlet molecular oxygen in supercritical fluids is currently being studied, with models based on radial distribution functions being applied to explain the observed kinetics.

Worrall, D.R. and Abdel-Shafi, A.A. "Photosensitized production of singlet oxygen and factors governing its decay in xenon and carbon dioxide supercritical fluids" *Journal of Photochemistry and Photobiology A: Chemistry* 186, 2007, 263-269.

Worrall, D.R., Williams, S.L. and Ganguly, T. "Ion-electron recombination on silica gel surfaces: experiment and modelling" *Photochemical and Photobiological Sciences* 5(9), 2006, 844-849
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Newcastle University
School of Chemical Engineering and Advanced Materials,

Photochemical studies in the School of Chemical Engineering and Advanced Materials, Newcastle University fall into the areas of Polymer photodegradation, Photocatalytic disinfection and detoxification of water and The application of nanoparticulate TiO₂ as an inorganic UV absorber for, e.g., cosmetics and sunblocks.

Polymer photodegradation studies use an *in situ* FTIR measurement to quantify the CO₂ generated during the irradiation of polymers. A study of a range of poly(ethylene) samples pigmented with different commercial TiO₂'s showed that the CO₂ measurement, which took 3-5 hours, correlated well with conventional measurements of carbonyl development which took many hundreds of hours. The convenience of the method allowed mechanistic details of polymer oxidation to be probed – for example the a dependence of oxidation rate was shown to vary as the square root of UV intensity. (Jin CQ, Christensen PA, Egerton TA and White JR. [Rapid measurement of polymer photo-degradation by FTIR spectrometry of evolved carbon dioxide](#), Polymer Degradation & Stability 91 (2006) 1086). A comparison of photodegradation of different polymers was reported at the 2007 Spring ACS meeting in Chicago. Water purification studies have shown that application of a small potential to TiO₂ photo-electrodes increases their efficiency for disinfection of E.coli suspensions. (Christensen PA, Curtis TP, Egerton TA, Kosa SAM [Photoelectrocatalytic and photocatalytic disinfection of E-coli suspensions by titanium dioxide](#) Applied Catalysis B-Environmental 41(2003) 371) and oxidation of nitrophenol. The possibly limiting effects of mass transport have been explored by comparative studies of dye decolouration by photocatalysis and photoelectrocatalysis (Egerton TA, Purnama H, Purwajanti S, [Decolouration of dye solutions using photoelectrocatalysis and photocatalysis](#), J. Adv. Oxidation Technol. 9 (2006) 79.) The effect of surface treatment on the properties of TiO₂ nanoparticulate sunblocks has been explored with respect to photogreying (Egerton TA, Kessell LM, Tooley IR, Wang L. [Photogreying of TiO2 nanoparticles](#), J. Nanoparticle Res.9 (2007): 251) and photo-oxidation, & photoreduction (Egerton TA, Mattinson JA [Comparison of photooxidation and photoreduction reactions on TiO2 nanoparticles](#) J. Photochem. Photobiol. A-Chem. 186 (2007): 115).

Terry Egerton
Newcastle University

Newcastle University
Molecular Physics Laboratory (MPL)

Research at MPL is subdivided into four main themes, though within them there exists a great deal of cross-fertilisation of ideas. The groups' expertise in synthesis, spectroscopy and computational chemistry combine to allow a wide range of modern photochemistry themes to be covered including: (i) molecular photonic devices, (ii) probing through bond electron transfer, (iii) understanding long range photo-effects and (iv) promoting directed electron transfer processes. The emphasis is rational design of molecular systems for specific purposes. One recent success has been the preparation of pyrene-based molecular dyads for potential imaging purposes using delayed fluorescence.

Prof. A. Harriman and Dr. A.C. Benniston
Newcastle University

University of Nottingham

The proposed research is to develop a novel fan/air cleaning device that could be used in buildings and industrial applications for the removal of gaseous, particulate and odorous pollutants. The proposed system will consist of a flexible fibre impeller coated with the photocatalyst titanium dioxide (TiO₂). The fibre impeller will be mounted on a shaft within a centrifugal fan casing and will be rotated by a direct drive, high efficiency motor. Using this arrangement, the flexible fibre fan has been shown to work efficiently as an air impeller. The device will provide both ventilation and air cleaning. Air cleaning will be achieved using the process of photocatalytic oxidation (PCO). PCO has strong potential to be a highly effective process for destroying air pollutants. A photocatalytic reactor operates at room temperature and chemically oxidises volatile organic pollutants, converting them primarily to carbon dioxide and water. To facilitate photocatalytic oxidation, the flexible fibre impeller will be bathed in ultraviolet light provided by a low energy, low cost, fluorescent UV-lamp. Furthermore, the system itself would have low energy consumption, as, unlike conventional air cleaning devices, there would be negligible pressure drop involved in its operation. It would therefore be energy efficient, compact and require little, or no maintenance. Its deployment would result in lower heating/cooling costs, improved indoor air quality and reduced emission of CO₂ to the environment.

Dr Xiaoli Ma
School of the Built Environment
University of Nottingham

Queen Mary, University of London

The Clean Materials Technology group based in UCL chemistry Department is headed by Dr. Jawwad A. Darr (j.a.darr@qmul.ac.uk) are using a novel method for synthesis and discovery of more efficient photocatalysts for splitting water. The group have developed Continuous Hydrothermal Flow Synthesis (CHFS) reactors for small and larger scale syntheses of highly crystalline inorganic nanomaterials. The process is a continuous way of making highly crystalline nanoceramics with unique properties in a few seconds. The group have developed and screened hundreds of doped titanias, and transition metal mixtures for photocatalytic decomposition of model pollutants. Current collaborations in solar cells are also being undertaken. For more information see group webpage www.qmul.ac.uk

Dr. Jawwad A. Darr
Queen Mary, University of London

Salford University

Researchers at Salford University have been active in the field of photocatalytic thin films for a number of years. They are focused on CVD (Chemical Vapour Deposition) routes to a wide range of thin film materials. Their initial work on photocatalytic thin films explored "self /easy clean" properties. Indeed, they were heavily involved in the very first work done with Pilkington on their Activ Glass product, which eventually became the world's first self clean glass product. They have extended this, in recent years, to biocidal coatings using photoactivity in combination

with other biocidal mechanisms. They have also collaborated with Prof. Mills at Strathclyde University in evaluating dye based tests for rapid photoactivity testing. A major thrust of their work has remained the chemical Engineering of CVD routes to growing thin films including photoactive films.

Prof. David Sheel
Managing Director CVD Technologies Ltd. and
Research Professor, Institute of Materials, Salford Univ.

Strathclyde University Physics Department

In the Physics Department at Strathclyde University photochemistry research is performed in the Biomolecular and Chemical Physics Group comprising:

The Photophysics Group (David Birch, Olaf Rolinski, Jan Karolin and Yu Chen)

Strathclyde University's Photophysics Group (<http://sensor.phys.strath.ac.uk/>) works on interdisciplinary molecular problems using time-resolved fluorescence techniques. Much of the group's work has found important outlets for knowledge transfer to industry. This includes founding the university spin-off manufacturer of fluorescence lifetime systems IBH, now part of the Horiba Jobin Yvon Group. Present emphasis of research is at the biomedical and nanometrology interface. A new Centre for Molecular Nanometrology has been set-up jointly with the Raman group from Strathclyde University's Chemistry Department to provide an integrated approach with fluorescence and ultrafast spectroscopy. Recent funding successes include an EPSRC and Scottish funding Council £5M Science and Innovation award in nanometrology for molecular science, medicine and manufacture.

Recent highlights:

1. The application of fluorescence lifetime sensing to novel assays for metabolic monitoring e.g. in-vivo glucose measurement. Recent review: *Fluorescence-based glucose sensors*. J C Pickup, F Hussain, N D Evans, O J Rolinski and D J S Birch. *Biosensors and Bioelectronics*. 20, 2555-65, 2005.
2. Developed multiphoton fs laser excited TCSPC fluorescence as a probe of microenvironment in terms the decay of anisotropy and stimulation of intrinsic fluorescence e.g. obtaining vacuum ultra-violet equivalent excitation of $\sigma \rightarrow \sigma^*$ transitions in hydrocarbons using 800 nm, green fluorescent protein, melanin and nanoparticle metrology. Review: *Fluorescence spectroscopy of biomolecular systems*. D J S Birch. *Spectrochimica Acta* 57, 2313-2336, 2001.
3. Dynamics of self-assembly of colloidal nanoparticles and pore structure of resulting ceramics derived from sodium silicate and silicon alkoxide sol-gels using new in-situ techniques for nanoparticle measurement. Recent paper: *pH tracking of silica hydrogel nanoparticle growth*. A Cleary, J Karolin and D J S Birch. *Appl. Phys. Letts.* 89, 113125-7, 2006.

4. FRET (fluorescence resonance energy transfer) theory is being developed in a new way to determine the donor-acceptor distance distributions without making a-priori assumptions as to its form. Applications include porous solids, metal ion sensors for water, self-assembled colloids and macromolecular structure and dynamics. First paper: *Determination of acceptor distribution from fluorescence resonance energy transfer: Theory and simulation*. O J Rolinski and D J S Birch. J.Chem. Phys. **112**, 8923-8933, 2000.
5. Demonstrated the first use of pulsed ultraviolet light-emitting diodes at 265 nm, 280 nm and 295 nm for exciting protein fluorescence. Recent paper: *Excitation of fluorescence decay using a 265 nm pulsed light-emitting diode: evidence for aqueous phenylalanine rotamers*. C D McGuinness, A M Macmillan, K Sagoo, D McLoskey and D J S Birch. *Appl. Phys. Letts.* **89**, 63901-3. 2006.

The Ultrafast Group (Klaas Wynne and Neil Hunt)

The Ultrafast Group (<http://bcp.phys.strath.ac.uk/ultrafast/>) operates the University's Femtosecond Research Centre and researches a range of chemical physics problems from small molecules to proteins. Recently, their work has concentrated on the terahertz dynamics of the condensed phase, including work on hydrogen-bonding liquids and the interactions of proteins with the surrounding solvent and on developing terahertz technology. This work has around £1.5M in active funding from EPSRC and the Leverhulme Trust. Latest work aims to observe the structural changes that occur at the active site of enzymes during their catalytic cycle. Supported by a £1M EPSRC Advanced Research Fellowship, a state-of-the-art femtosecond two-dimensional infrared (2D-IR) spectrometer is being constructed that will be capable of following reactions and the structure of the active site in real time in unprecedented detail.

Recent highlights:

1. The group has recently reported the observation of fractional Stokes-Einstein-Debye relaxation in liquid N-methylacetamide (NMA), a peptide linkage model compound. This phenomenon, arising from heterogeneities in NMA due to hydrogen-bonded chain formation causing the decoupling of rotational relaxation from the shear viscosity, is highly unusual in a 'normal' liquid and is generally associated with fluorescence measurements of large dye molecules in glass-forming liquids. See "*The effect of temperature and solvation on the ultrafast dynamics of N-methylacetamide*" Hunt, NT; Wynne, K, *Chem. Phys. Lett.* **431**, 155-159 (2006).
2. The ultrafast dynamics associated with the α -helix to random coil transition of peptide molecules have been studied. Secondary-structure dependent changes in the timescale of the sub-picosecond dynamics due to peptide-solvent Hydrogen bonding are consistent with the first observation of the proposed Lubricant of Life mechanism in which solvent-solute dynamics directly influence protein structure. See "*The Dynamics of Water-Protein Interaction Studied by Ultrafast Optical Kerr-Effect Spectroscopy*", Hunt NT; Kattner, L; Shanks, RP; Wynne K, *J. Am. Chem. Soc.* **129**, 3168-3172 (2007)
3. Nanostructured surfaces have been developed for the generation of ultrafast terahertz pulses. Excitation of surface plasmon absorptions in gold-coated gratings leads to emission of electrons and production of terahertz-frequency pulses. The ability to produce high power terahertz pulses will bring significant benefits for many fields of research,

including the study of the dynamics of liquids and protein systems. "*Terahertz-pulse emission through laser excitation of surface plasmons in a metal grating*", Welsh, GH; Hunt, NT; Wynne K, *Phys. Rev. Lett.* **98**, 026803 (2007)

4. The contribution of solvent-solute hydrogen bonding to the terahertz Raman spectrum of solutions has been studied. This first direct spectroscopic observation of vibrational modes of hydrogen bonds provides a basis for interpreting terahertz spectra of protein and enzyme systems. "*Inter- and intramolecular hydrogen bonding in phenol derivatives: A model system for poly-L-tyrosine*", Hunt, NT; Turner, AR; Wynne, K, *J. Phys. Chem. B* **109**, 19008-19017 (2005)

Prof. David Birch
Head of Department of Physics
University of Strathclyde

Swansea University

Swansea University has a number of Doctorate students working with Akzo Nobel, BASF and Corus Group on projects to do with organic coating photodegradation funded through our EngD programme. Highlights include some rapid testing techniques for titania grades used in paints which can reasonably reliably rank durability in 24-48 hours. Also some interesting speciation work on photodegradation products (for example materials of unknown toxicity coming out of commercial titania containing sun blocks!!)

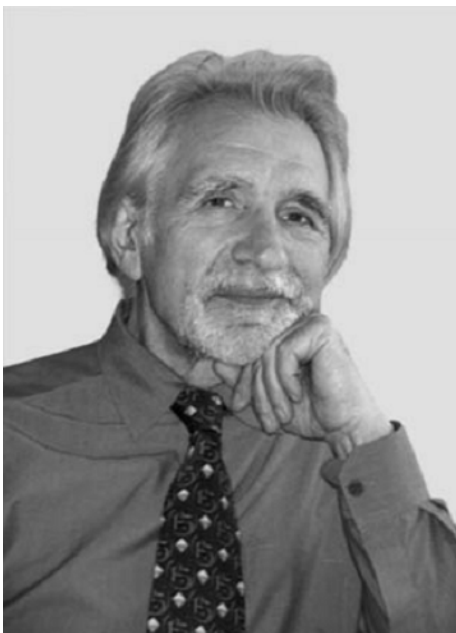
Swansea has also just started a big project on DSSCs with ICL, Bath and Bangor. The aim to produce low cost metal mounted PVs for walling and roofing. Again Corus is the industry partner with funding from EPSRC. The main motivation for this work is that Corus produce 100 million square metres of roofing and walling per annum in the UK and at the moment this has no other function than protection and decoration. Hence incorporating even a low efficiency PV into these materials is attractive.

Dr David Worsley
Engineering School
Swansea University

PERSONAL NEWS

70th Birthday of Prof. Mikhail Alfimov

Scientific School of Academician Mikhail V. Alfimov.



The seventieth birthday of Academician Mikhail Vladimirovich Alfimov, a prominent physical chemist, well-known specialist in the field of molecular photonics, chemical physics of supramolecular and nanosized systems, and the author of more than 500 publications, have been on July 6, 2007. The scientific achievements of Prof. M. V. Alfimov were recognized by the award of the State Prize, the Friendship Order, the Order of the Service to the Fatherland, the French Legion of Honor, and the Cross for the Service to Federal Republic of Germany. During more than forty-five years of his scientific activity, Alfimov created a unique scientific school, from which tens of well-known Russian scientists graduated.

Now M.V. Alfimov is a head of the Photochemistry Center - a unique research institute of the Russian Academy of Sciences, in which experimental and theoretical studies on the structure, dynamics, and photonics of molecules and supramolecular and nanosized systems are carried out. Molecular solutions and ensembles of complexes, nano- and microstructures on surfaces (including Langmuir-Blodgett films) and in liquid and solid solutions are the main subjects of research. Systems composed of molecules of aromatic hydrocarbons, aromatic amines, spiropyrans, spironaphthaxazines, chromenes, styryl and polymethine dyes, crown-containing dyes, cyclodextrines, etc. are also subjects of the study.

The research works at the Photochemistry Center are focused on the establishment of the interrelation between the structure of supramolecular and nanosized systems and their linear and nonlinear optical properties, the effectiveness of the photochemical reactions, photoinduced electron transfer, photoisomerization, photocyclization, etc.

The aim of the studies carried out at the Photochemistry Center is the revealing the principles of controlling the optical and photochemical properties of supramolecular nanostructures via their organization. Materials and devices for optical information recording, photonic crystals, materials with nonlinear optical properties, photovoltaic and electroluminescent materials, and chemical and biological sensors are potential fields for the application of the results of scientific research.

Currently, a new field of investigations, the photonics of supramolecular and nanosized systems has been developed at the Photochemistry Center. These investigations are carried out in cooperation with many Russian and foreign scientific centers, the Institute of Problems of Chemical Physics, Frumkin Institute of Physical Chemistry and Electrochemistry, Faculties of Physics and Chemistry of Moscow State University, Zelinsky Institute of Organic Chemistry, Shemyakinn Ovchinnikov Institute of Bioorganic Chemistry, and Kurnakov Institute of General and Inorganic Chemistry (Russia); University of Texas in Austin, North Carolina State University, and Florida State University (the United States); Max-Planck-Institut für Biophysikalische Chemie, FR Organische Chemie der Universität der Saarlandes, and am Engler-Bunte Institute der Universität Karlsruhe (Germany); University of Umea (Sweden); University of Durham and University of York (United Kingdom); Università degli Studi di Bologna (Italy); University of Bordeaux I and University of Marseille (France); etc. Several studies at the Photochemistry Center were fulfilled within the frame-work of agreements with Corning Co. and Samsung.

The investigations carried out during the last decade were supported by the international and Russian foundations such as RFBR, MNTTs ISF, INTAS, CRDF, DFG, Royal Society, CNRS, and NWO.

The Photochemistry Center is recognized as one of the world leading center of research in the photonics of organic nanostructures, organizes international conferences and workshops on this subject and is a head organization in the programs of the Russian Academy of Sciences in the field of nanosized organic and hybrid organic-inorganic structures. M. V. Alfimov is an Editor-in-Chief of the scientific journals *High Energy Chemistry* and *Russian Nanotechnologies*.

A great deal of attention is paid to the training of specialists, bachelors, masters, and PhD students corresponding to the profile of the Photochemistry Center from leading Moscow Universities: Moscow Physico-Technical Institute, Moscow State University, Mendeleeev University of Chemical Technology (International Higher College for Chemistry of Composite Materials), and Lomonosov Moscow State Academy of Fine Chemical Technology. More than fifty students from different Russian Universities are trained at the Center every year.

Prof. Vladimir Razumov
Vice director of the Institute of Problems of Chemical Physics

TECHNICAL REPORT

Practical examples on the correct representation of electronic spectra.

Gonzalo Angulo¹

*Physical Chemistry Department, Sciences II, University of Geneva
30, Quai Ernest Ansermet CH-1211 Geneva, 4 Switzerland*

Abstract.

Stationary light absorption and fluorescence of molecules in diluted liquid solutions is currently widely used in research and applications. Most of the commonly used spectroscopic devices make use of wavelength resolved gratings while the appropriate spectra representation has to be done in the inversely proportional energy scale. The correct way to represent the spectra in order to extract physically meaningful parameters is known for a long time, but there are still many examples of unfortunate data handling. This paper complements a former one with real examples and discusses under which circumstances and for which cases special attention has to be paid to the data processing.

Introduction.

The appropriate way to represent the spectra of absorption and emission of light in the UV-VIS-NIR range due to electronic transitions in polyatomic molecules in solution is known for very long now.[1-3] Starting from the electromagnetic wave theory and the Einstein coefficients, Förster already in the fifties derived the relationship between the transition dipole moments for the absorption and fluorescence and the respective spectra. Not in vain, his model for the dipole-dipole mechanism of energy transfer contains this relationship.[1] Following this seminal work, Strickler and Berg derived their well known expression for the radiative or intrinsic lifetime of the excited state.[4] Even in the calculation of the energy of charge transfer bands Förster's expressions found application by relating the energy gap law and the spectral shape.[5]

Despite all the former cited works, there are still many examples in the scientific literature of unfortunate handling of the electronic spectra. Absorption and fluorescence apparatuses usually record spectra in the wavelength scale which are then very often directly used to obtain transition energies, dipole moments or directly compared to each other in order to check whether the mirror symmetry rule is fulfilled. Very often these spectra are used to extract zero-zero energies, when evaluating excited state reaction energies, or the Stokes shift, when dealing with solvatochromism.

In a former paper, we already presented the theoretical justification of what we there called Transition Dipole Moment (TDM) representation. Simulations, which were based on the displaced distorted harmonic oscillator allowed for an estimation of the error committed in the evaluation of fluorescence maxima, zero-zero energies and the Stokes shift, when using directly the unmodified wavelength spectra.[6] In the present communication we have taken about 100 spectra of real samples from a well known online database (PhotochemCAD) [7] to perform the same comparison in order to discuss the issues of a bad spectral manipulation and the possible consequences. Some special cases are individually discussed for their special interest. Finally, some more calculations have been performed to gain further insight in the deviations in solvatochromism studies arising from inappropriate spectra manipulation.

¹ On leaving to the Institute of Physical Chemistry, Polish Academy of Sciences, Warsaw (Poland).

Methodology.

Making use of the available spectra from [7], which are given in the wavelength scale, and supposing that the fluorescence spectra have been corrected for the fluorometer response, they have been represented in wavenumbers by simply inverting the wavelength in the case of the absorption spectra, and by multiplying the fluorescence spectra by the square of the wavelength,

$$\varepsilon(\lambda) = \varepsilon(\tilde{\nu})$$

$$\left. \begin{aligned} \varphi(\tilde{\nu}) = \varphi(\lambda) &\Rightarrow |F(\tilde{\nu})d\tilde{\nu}| = |F(\lambda)d\lambda| \\ \tilde{\nu} = \lambda^{-1} &\Rightarrow d\tilde{\nu} = -\lambda^{-2}d\lambda \end{aligned} \right\} F(\tilde{\nu}) \propto \lambda^2 F(\lambda).$$

It has been shown, that the transition dipole moments of absorption and fluorescence, or in other words, the transition probabilities, are proportional to the following [6]:

$$\left| \vec{M}_{ub \rightarrow la} \right|^2 \propto \tilde{\nu}^{-3} F(\tilde{\nu}) = I(\tilde{\nu}) \quad \text{and} \quad \left| \vec{M}_{la \rightarrow ub} \right|^2 \propto \tilde{\nu}^{-1} \varepsilon(\tilde{\nu}) = A(\tilde{\nu}),$$

where the subscripts stand for the transition from the upper electronic level in the b vibrational state to the lower electronic level in the a vibrational state, and vice versa for the fluorescence and absorption, respectively.

Thus, the conversion of absorption and fluorescence spectra into their TDM equivalents requires division by wavenumbers for the former and division by wavenumbers to the fifth for the latter.

Table 1: Chromophores and solvents corresponding to the absorption and fluorescence spectra analyzed in Figures from 1 to 4, as given by the database of reference [7].

1 7-Methoxycoumarin-4-acetic acid / methanol	27 Zinc tetramesitylporphyrin / toluene	53 N,N'-Difluoroboryl-1,9-dimethyl-5-phenyldipyrrin / toluene	79 Perylene / cyclohexane
2 9,10-Bis(phenylethynyl)anthracene / cyclohexane	28 Zinc tetraphenylporphyrin / toluene	54 N,N'-Difluoroboryl-1,9-dimethyl-5-(4-iodophenyl)-dipyrrin / toluene	80 Phenol / hexane
3 Indocarbocyanine (C3)dye / methanol	29 Acridine orange / basic ethanol	55 9,10-Diphenylanthracene / cyclohexane	81 Phenylalanine / water
4 Oxacarbocyanine (C3)dye / ethanol	30 Acridine yellow / ethanol	56 1,2-diphenylacetylene / ethanol	82 Phthalocyanine / chloronaphthalene
5 Thiocarbocyanine (C3)dye / ethanol	31 4-Dimethylamino-4'-nitrostilbene / benzene	57 1,4-diphenylbutadiene / hexane	83 Pinacyanol iodide / metanol
6 Thiocarbocyanine (C3)dye propanol	32 Anthracene / cyclohexane	58 1,4-diphenylbutadiyne / ethanol	84 Piroxicam / hexane
7 Indodicarbocyanine (C5)dye / methanol	33 Auramine O / water	59 1,6-Diphenylhexatriene / cyclohexane	85 Porphin / toluene
8 Oxadicarbocyanine (C5)dye / ethanol	34 Benzene / cyclohexane	60 Eosin Y / basic ethanol	86 Proflavin / water pH 7
9 Thiadicarbocyanine (C5)dye / ethanol	35 Biphenyl / cyclohexane	61 Ethyl p-dimethylaminobenzoate / ethanol	87 Pyrene / cyclohexane
10 Indotricarbocyanine (C7)dye / ethanol	36 Chlorophyll a / methanol	62 Fluorescein / ethanol	88 Quinine sulfate / 0.05 M H2SO4
11 Oxatricarbocyanine (C7)dye / ethanol	37 Chlorophyll a / diethyl ether	63 Fluorescein / basic ethanol	89 Quinine sulfate / 0.5 M H2SO4
12 Tetrakis(2,6-dichlorophenyl)porphyrin / toluene	38 Chlorophyll b / diethyl ether	64 Hoechst 33258 / N,N-dimethylformamide	90 Rhodamine 123 / ethanol
13 Diprotonated-tetraphenylporphyrin / chloroform + HCl	39 Coumarin 1 / ethanol	65 Hoechst 33258 / water	91 Rhodamine 6G / ethanol
14 Magnesium phthalocyanine / propanol	40 Coumarin 30 / acetonitrile	66 Lucifer yellow CH / water	92 Rhodamine B / ethanol
15 Magnesium phthalocyanine / pyridine	41 Coumarin 314 / ethanol	67 Merocyanine 540 / ethanol	93 Riboflavin / ethanol
16 Magnesium octaethylporphyrin / dichloromethane	42 Coumarin 343 / ethanol	68 2-Methylbenzoxazole / cyclohexane	94 Rose bengal / basic ethanol
17 Magnesium octaethylporphyrin / toluene	43 Coumarin 6 / ethanol	69 Naphthalene / cyclohexane	95 Squarylium dye III / dichloromethane
18 Magnesium tetramesitylporphyrin / toluene	44 Cresyl violet perchlorate / ethanol	70 Nile blue / ethanol	96 Stains all / etanol
19 Magnesium tetraphenylporphyrin / toluene	45 Cryptocyanine / ethanol	71 Nile blue / methanol	97 Stilbene / hexane
20 Octaethylporphyrin / benzene	46 Crystal violet / glycerol	72 Nile Red / dioxane	98 Sulforhodamine 101 / ethanol
21 POPOP / cyclohexane	47 Dansyl glycine / dioxane	73 7-Benzylamino-4-nitrobenz-2-oxa-1,3-diazole / ethanol	99 Tetra-t-butylazaporphine / chlorobenzene

22 2,5-Diphenyloxazole / cyclohexane	48 4',6'-Diamidino-2-phenylindole / dimethylsulfoxide	74 Tetrakis(o-aminophenyl)porphyrin / toluene	100 Tetra-t-butyl-naphthalocyanine / chlorobenzene
23 Tetramesitylporphyrin / toluene	49 4',6'-Diamidino-2-phenylindole / water	75 Oxazine 1 / methanol	101 toluene / cyclohexane
24 Tetrakis(2,6-dichlorophenyl)porphyrin / toluene	50 4-(dicyanomethylene)-2-methyl-6-(p-dimethylaminostyryl)-4H-pyran / acetonitrile	76 Oxazine 170 / methanol	102 Tris(2,2'-bipyridyl)ruthenium(II) / water
25 Zinc phthalocyanine (ZnPc) / pyridine	51 4-(dicyanomethylene)-2-methyl-6-(p-dimethylaminostyryl)-4H-pyran / methanol	77 p-Quaterphenyl / cyclohexane	103 Tryptophan / water
26 Zinc octaethylporphyrin / toluene	52 N,N'-Difluoroboryl-1,9-dimethyl-5-[(4-(2-trimethylsilylethynyl)phenyl)dipyrin] / toluene	78 p-Terphenyl / cyclohexane	104 Tyrosine / water

The differences between the maxima corresponding to the transition between the same states, of the two ways of representing the spectra have been computed for both the absorption and fluorescence for each of the about 100 examples, and plotted against the value of the maxima in the TDM representation. In some cases, special attention has to be paid to too noisy data or to multiple peaks of similar height. In the latter cases, it can happen that the most intense band moves from one to another peak of a vibrational progression, leading to unreasonable results. These effects have been corrected, and all the differences are computed using the same vibronic transitions.

The calculations performed for the simulations have been described in detail in a previous paper.[6]

Results.

Figure 1 represents the difference between the absorption in the TDM and the untransformed representation (but already in the wavenumbers scale) while figure 2 shows the same for the fluorescence spectra.

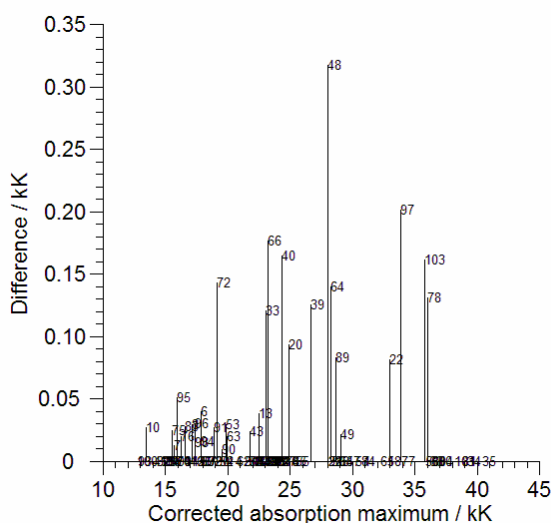


Figure 1: Differences between the TDM and the NON-TDM representations in the absorption maxima collected from the database of reference [7], against the maxima extracted from the TDM representation. See Table 1 for a list of the substances corresponding to the plotted numbers.

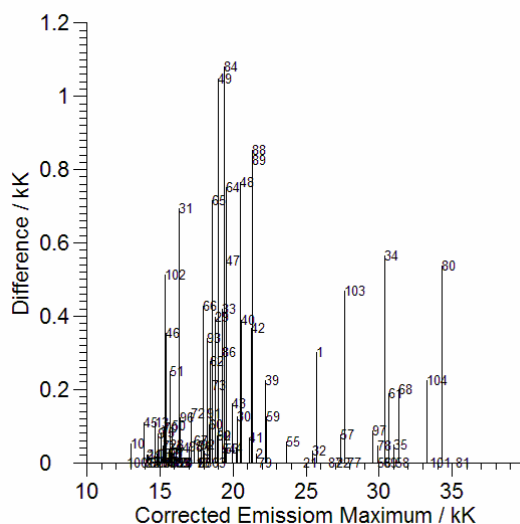


Figure 2: Differences between the TDM and the NON-TDM representations in the fluorescence maxima collected from the database of reference [7], against the maxima extracted from the TDM representation. See Table 1 for a list of the substances corresponding to the plotted numbers.

Note that these differences are always positive since the effect of the correction is to shift the spectra to the red, i.e., to lower energies. Obviously, the extent of the error in the absorption spectra is much smaller than in the case of the emission spectra. Moreover, despite the observations made in the simulations in the previous paper, the deviations are not clearly more important for compounds absorbing at lower energies. In fact, the most pronounced effects are found for very broad spectra, giving rise to deviations as high as 0.3 kK^2 (150% of the thermal energy under usual working conditions). One should be especially cautious with spectra showing a distinct vibrational progression: the relative intensity of different vibronic bands may be inverted, and the spectral maximum artificially shifted. Normally, the purpose of a spectral analysis is to compare similar transition bands, i.e. the same vibronic band should be used for the comparison in different environmental conditions or to measure the transition energy. In the case of the fluorescence spectra the deviations are even bigger, reaching 1 kK, about 5 times the thermal energy. Now, a certain tendency when shifting the spectra to the red can be observed, in accordance with the previous simulations. However, the effect of the spectral presentation is, as in the case of the absorption spectra, a function of both, spectral shape and position.

² kK stands for kiloKaiser. $1 \text{ kK} = 1000 \text{ cm}^{-1}$.

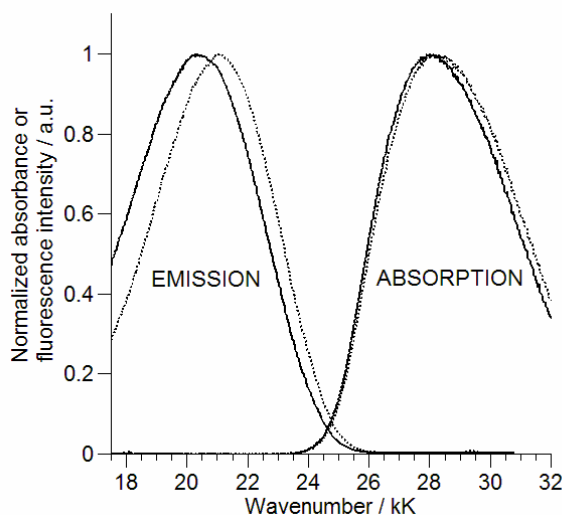


Figure 3: Absorption and fluorescence spectra of 4',6-diamidino-2-phenylindole / DMSO in the TDM (solid lines) and NON-TDM representations.

A demonstrative example of absorption and fluorescence spectra in both representations is given in Figure 3. This is a very special case because of the enormous width of the bands. It corresponds to the point 48 (4',6-diamidino-2-phenylindole / dimethylsulfoxide). As can be seen, the spectra are not located at low energies, and still the deviations from one to the other representation are quite important. To better see the influence of a wrong representation of the electronic spectra on their shape, we have chosen Coumarine 6 in ethanol (point 43, see Figure 4) and transposed the absorption spectrum to $\tilde{\nu}'_{\text{abs}} = 2\tilde{\nu}_{0-0} - \tilde{\nu}_{\text{abs}}$, where $\tilde{\nu}_{0-0} = (\tilde{\nu}_{\text{abs}}^{\text{max}} + \tilde{\nu}_{\text{em}}^{\text{max}})/2$ is the absorption/emission average 0-0 transition energy. In the right panel the NON-TDM representation clearly shows that the transposed absorption spectrum does not coincide with the emission band. Once correctly represented (left panel) the superposition between both absorption and fluorescence emission spectra is very good and it can be safely concluded that this molecule in this solvent indeed shows mirror symmetry. Not representing correctly the spectra could lead to the conclusion that, for example, the Strickler-Berg equation is not applicable in the present case, or that the changes in the molecular geometry upon electronic excitation are very important. Hence, even if the energy differences between both representations are not very high, as it is the case for point 43, the spectral shape can be severely distorted in the NON-TDM representation and thus give rise to erroneous interpretations of the spectra at hand.

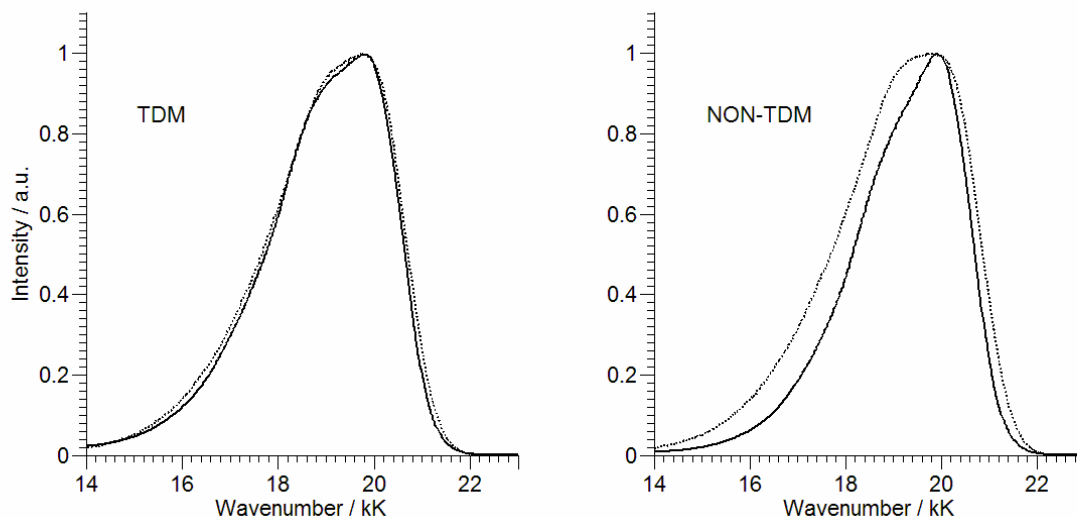


Figure 4: Fluorescence (solid lines) and absorption spectra of coumarin 6 in ethanol in TDM and NON-TDM representations. The absorption spectrum has been transposed to check the mirror symmetry between both spectra.

In our previous work [6] on the differences between these ways of representing the electronic spectra, we did not explicitly analyse the errors in the slopes of the change of the Stokes shift against the Lippert solvent function [8] $F(n_D^2, \epsilon) = \frac{\epsilon - 1}{2\epsilon + 1} - \frac{n_D^2 - 1}{2n_D^2 + 1}$ where n_D^2 is the square of the refractive index of the solvent at the D line of sodium, and ϵ the dielectric constant of the medium. In the frame of the Lippert model, the Stokes shift is equal to

$$\Delta \tilde{\nu} = \tilde{\nu}_{abs}^{max} - \tilde{\nu}_{em}^{max} = \tilde{\nu}_{abs,0}^{max} - \tilde{\nu}_{em,0}^{max} + \frac{1}{2\pi\epsilon_0 hc} \frac{(\mu_e - \mu_g)^2}{r^3} F(n_D^2, \epsilon)$$

where the subscript 0 stands for the values in the gas phase, e and g for the excited and ground state respectively, μ for the dipole moment and r for the Onsager cavity radius in the reaction field created by the solvent continuum. We are not going to discuss the merits and pitfalls of this model and its uses, but it has to be recognized as a widespread tool for the analysis of solvatochromism. Regarding the way of representing absorption and emission spectra in order to perform such analysis and extract from the slope the change in the dipole moment upon excitation, we previously concluded that the error made using the NON-TDM representation is negligible.[6] This is absolutely true for spectra that do not show any change in shape on changing the solvent. But, if for example, the width of the spectra increases with the solvent function, some deviations may be appreciated. Furthermore, it is no longer convenient to take the spectral maxima but the centre of gravity of the spectra,[9] given by

$$\tilde{\nu}_{abs}^{cg} = \frac{\int A(\tilde{\nu}) \tilde{\nu} d\tilde{\nu}}{\int A(\tilde{\nu}) d\tilde{\nu}} \quad \text{and} \quad \tilde{\nu}_{em}^{cg} = \frac{\int I(\tilde{\nu}) \tilde{\nu} d\tilde{\nu}}{\int I(\tilde{\nu}) d\tilde{\nu}}.$$

We have performed calculations with the displaced-distorted harmonic oscillator, as described previously, changing the solvent function from 0 to 0.4, the usual range for common solvents. The width of the spectra has been changed by varying the Gaussian width: $w = 2 + 1.875 F(n_D^2, \epsilon)$ kK. Figure 5 shows the results with both ways of representing the spectra and extracting either the maxima or the centre of gravity. All four curves show different slopes, and only the upper

one, using the centre of gravity of the bands obtained from the TDM representation, gives the accurate slope. The slope is known in the calculations from the parameters used, collected in Table 2, and it is equal to 3.9 kK.

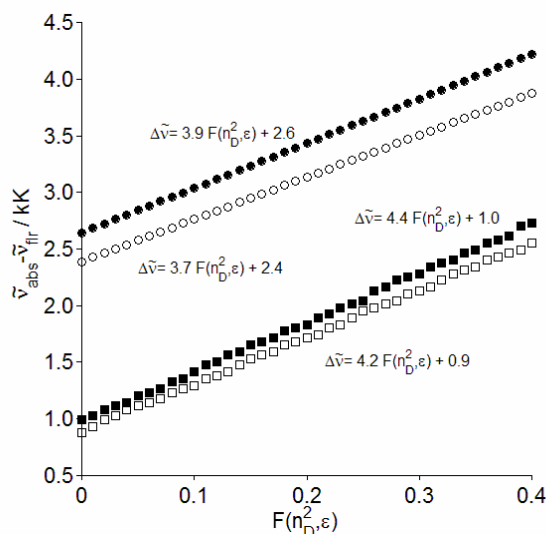


Figure 5: Stokes shift dependence on the Onsager solvent function (see text for the spectra simulation details). Open symbols: data extracted from the NON-TDM representation. Full symbols: data from TDM representation. Squares: shifts obtained from the spectra maxima. Circles: shifts obtained from the centers of gravity. The equations stand for the best linear fit for each data set.

Table 2: Parameters used in the calculations with the displaced-distorted harmonic oscillator employed in Figure 5.

$\tilde{\nu}_{0-0}$ is the 0-0 electronic transition energy, ω is the Gaussian width of the spectra, $\tilde{\nu}_{\text{vib}}$ is the vibrational frequency, and a and R are proportional to the displacement and the distortion in the two electronic level system.

$\tilde{\nu}_{0-0} / \text{kK}$	ω / kK	$\tilde{\nu}_{\text{vib}} / \text{kK}$	a	R	m_g / D	m_e / D	$r / \text{\AA}$	$F(n_D^2, \epsilon)$
1.5	2-2.75	1.0	1.51	1.75	3	10	5	0.0-0.4

Summary.

It has been shown through experimental examples that the discrepancy between the energies extracted from the absorption and emission spectra if wrongly handled, are not small. It depends very much on the shape, the width and the energy of the spectra. In general, for the absorption spectra, the bandwidth is most influential on the error made when using a NON-TDM representation, while in the fluorescence emission the position of the spectrum also plays a major role. It is of special interest the case of coumarin 6. Even if the quantitative error in the NON-TDM spectra is small, their shapes are so distorted that the mirror symmetry between absorption and fluorescence is lost.

Additionally, the simulations performed show that if the spectral width changes from one solvent to another, some minor errors can be encountered in the extraction of the dipole moment change upon excitation. Therefore, it is safer to extract the centre of gravity of the absorption and fluorescence spectra represented in the TDM representation for solvatochromism studies, rather than using the corresponding maxima.

Acknowledgements.

The author is very grateful to Prof. Eric Vauthey, Jakob Grilj (University of Geneva) and Arnulf Rosspeintner (TU Graz) for helpful discussions and their comments on the manuscript. This work has been supported by the University of Geneva.

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PUBLICATIONS

Abstracts of Theses in Photochemistry

Tatjana V. Sokolova

Spectral luminescent and photochemical properties of methylphenols and dihydroquinolines in different media

Tomsk State University; 1, Novosobornaja sq., Tomsk, 634050, Russia
PhD thesis (in Russia), November 2006, Tomsk State University
Supervisor: Prof. Irina V. Sokolova

The fluorescent properties of different phenol compounds in different pH values under UV-irradiation were studied.

Objects: 2-methylphenol (2-MP), 4-methylphenol (4-MP), 2-amino-4-methylphenol (2-A-4-MP), 6-hydroxy-2,2,4-trimethyl-1,2-dihydro-quinoline (6-OH-DHQ) and 8-hydroxy-2,2,4-trimethyl-1,2-dihydro-quinoline (8-OH-DHQ).

Methods. The spectral-luminescent and photochemical properties of the neutral and ionic forms of methylphenols (MP) and of the neutral form of hydroxy substituted 2,2,4-trimethyl-1,2-dihydro-quinolines (DHQ) in water and different solvents are studied by method of electron spectroscopy. The interpretation of obtained data was carried out by quantum-chemical calculations, in particular, by means of intermediate neglect of differential overlap (INDO) with parameterization method.

Radiation sources. The following sources of radiation were used: 1) low pressure mercury lamp; 2) exciplex lamps on KrCl^* ($\lambda \sim 222$ nm), XeBr^* ($\lambda \sim 283$ nm) and XeCl^* ($\lambda \sim 308$ nm) molecules; 3) pulsed excimer KrCl -laser ($\lambda = 222$ nm), XeCl -laser ($\lambda = 308$ nm); 4) Nd:YAG-laser (4th harmonica, $\lambda = 266$ nm). The choice of radiation sources was caused by the necessity of selective excitation of molecule of interest in its absorption bands. The checking of photoreaction course of MP and DHQ molecules was conducted by monitoring of changes in long-wavelength UV absorption spectra of the initial compounds and reaction products. Spectral and kinetic parameters of short-living intermediate species were measured by pulse photolysis method with a resolution time of 10 μs .

Results

1. The spectral-luminescent properties of the neutral and ionic forms of MP and of the neutral form of DHQ in water and aqueous micellar solutions.

1.1. It is shown theoretically that the long-wavelength absorption band of 4-MP corresponds to the $S_0 \rightarrow S_1 \pi\pi^*$ -type electron transition having low intensity (oscillator strength $f = 0.03$). The short-wavelength spectral band is formed by two electron transitions: $S_0 \rightarrow S_2 \pi\sigma^*$ -type ($f = 0.001$) and $S_0 \rightarrow S_3 \pi\pi^*$ -type ($f = 0.15$), which is formed without participation of the OH group of the 4-MP molecule. These states are formed by molecular orbitals localized on carbon atoms of the aromatic ring. Experimentally, the fluorescence quantum yield (ϕ) of 4-MP in water was determined ($\phi = 0.2$).

1.2. It is shown theoretically and experimentally that the incorporation of NH_2 group to the 4-MP molecule leads to decreasing of energies and electronic states S_1 and S_3 , increasing oscillator strength of transitions S_2 and S_7 , and forming absorption band of 2-A-4-MP in the middle spectral range (42000 cm^{-1}). Moreover, the fluorescence quantum yield of 2-A-4-MP in

water decreases ($\phi = 0.004$) because of the high efficiency of S_1T_3 conversion. Under excitation of the absorption spectrum of 2-A-4-MP in the middle spectral range the degradation channel of excitation energy through a system of triplet states arises under excitation of the absorption spectrum of 2-A-4-MP (fluorescence quenching) have place.

1.3. A comparison between forming of anionic forms of 2-A-4-MP and MP. It has been found that the anionic forms of 2-A-4-MP in water-alkali solutions forms easily than those of 4-MP. Under excitation to S_1 state of MP, the neutral and acid properties of 4-MP are lower in comparison with 2-MP. Anionic MP has low fluorescent output because of the high efficiency of the intercombination conversion in MP. Under excitation to S_1 state of 2-A-4-MP, the proton-acceptor properties of 2-A-4-MP are lower in comparison with MP.

1.4. The spectral-luminescent properties of MP in case of surfactants presence in water have been investigated. Using of aqueous micelle solution has allowed to change the reactivity of MP in comparison with aqueous solutions of MP. The proton-donor properties of MP in the presence of the CTAB and SDDS micelles in the ground electronic state decreases in comparison with aqueous solutions. In the presence of the triton X100 micelles, the anion forms of MP were not observed in the ground and excited states. The anion forms of 4-MP in the ground and excited states were detected in aqueous alkaline solutions only in the presence of cation surfactant micelles. Under excitation to S_1 state, the interaction of MP with the alkali in the aqueous micelle solutions was stronger than with the acid.

1.5. The spectral-luminescent properties of 6-OH-DHQ and 8-OH-DHQ in water, hexane, methyl and isopropyl alcohol were studied. It is shown, that formation of intra- and intermolecular hydrogen bonding exerts influence on the spectral characteristics of DHQ.

2. Photolysis of MP. Influence of mediums acidity and excitation energy on the phototransformation efficiency.

2.1. The efficiency of MP photodecay in neutral medium is highest under UV irradiation by KrCl excilamp (under excitation to S_3 state of molecules). In acid and neutral media (where the molecules are in ionic form) the highest efficiency of photodecay have place under UV irradiation by XeBr-excilamp (under excitation to S_1 state).

2.2. Incorporation of NH_2 group to the 4-MP molecule increases the reactivity of molecule: the photodecay efficiency increases in a following row: 2-MP < 4-MP < 2-A-4-MP. The photolysis products of neutral aqueous solutions of 2-MP and 4-MP under UV irradiation by all lamps has fluorescence in the wavelength range with maximums at 350 and 410 nm.

3. The influence of solvents on photochemical processes in 6-OH-DHQ and 8-OH-DHQ solutions.

3.1. The schemes of photoinduced reactions occurring in 6-OH-DHQ and 8-OH-DHQ methanol and water solutions are proposed. It was shown that the direction and the kinetic parameters of the photoreactions depend on the position of the hydroxyl group on the aromatic ring. In MeOH solution for 6-OH-DHQ and for 8-OH-DHQ the photoaddition of the solvent molecule to the double bond of DHQ dominates. However, the raised acidity of the excited state leads to the formation of transient species which gives by-products as the result of transformations of the excited DHQ phenolate ion. These processes are stimulated in aqueous solutions owing to the possibility of the acid–neutral transformations between intermediates formed from different excited OH-DHQ molecules.

Conclusions

The research results are recommended for use in the fluorescence analysis, for example, in a task of control the purification of water from phenol impurities. As a practical matter, the most important result is the experimental fact that the most efficient phototransformations of neutral aqueous solutions of 2-MP, 4-MP and 2-A-4-MP are have place under theirs excitation into short-wavelength absorption band. Increasing or decreasing of pH medium (pH = 11.45 or

pH = 0.25) leads to changing of the electron-excited states of molecules. Therefore in these cases it is necessary to apply the long-wavelength absorption band excitation for photolysis intensification.

Gabriella Ginocchetti

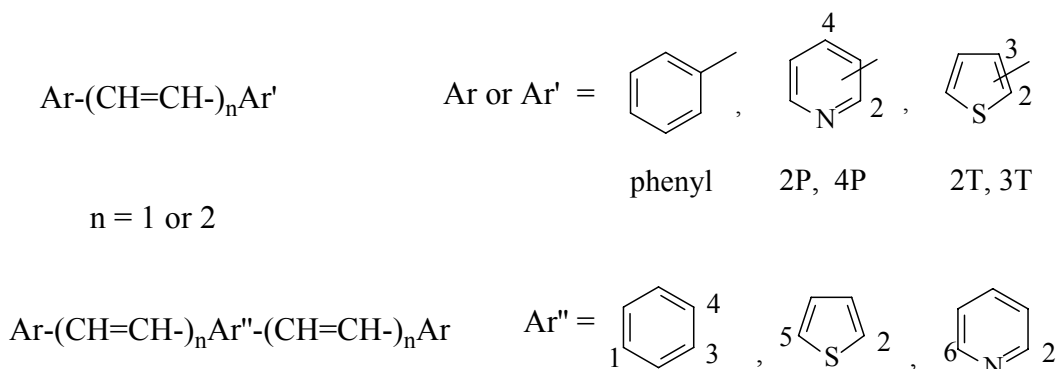
Excited state relaxation of geometrical and conformatuional isomers of diarylolefins

Dipartimento di Chimica, Università di Perugia, 06123 Perugia, Italy

Ph. D. Thesis (in English), February 2007

Research Advisors: Anna Spalletti, Ugo Mazzucato

This research work dealt with a study of the excited state properties of some thio- and aza-derivatives of stilbene-like molecules.



The effect of the unsaturated chain length and positional isomerism on the competition between radiative, non-radiative and reactive deactivation pathways and on the role of conformational isomerism in the photobehaviour has been deeply investigated.

Thio-derivatives

The substitution of benzene rings with thiophene rings in stilbene-like molecule generally induces an increase of the intersystem crossing rate parameter (k_{ISC}) due to the heavy-heteroatom effect, opening the way to photoisomerization in the triplet excited state. Moreover, a role of rotamerism in the photobehaviour is generally found when the thiophene ring is substituted in the 3-position, due to the presence of ground-state conformational equilibria among species with comparable abundance.

In the case of symmetric and asymmetric thienyl derivatives of ethenes and butadienes, the photobehaviour remains rather similar to that of the hydrocarbon (the fluorescence yield is low, of the order of 1-5%, and the photoisomerization yield is substantial, of the order of 35-45%), but the increase of k_{ISC} leads to a change in the photoisomerization mechanism from singlet (for 3-styrylthiophene) to mixed [for 1,2-di-(3'-thienyl)ethene and asymmetric dienes] and to triplet [for 1,2-di-(3'-thienyl)butadiene]. The length of the unsaturated chain and its position with respect to the heteroatom can have a substantial effect on the relative energy of the two lowest excited singlet states of A_g and B_u parentage. The two states are so close in the dienes that the experimental conditions (solvent polarizability, temperature, etc.) or structural factors (nature of the aryl groups, position of the heteroatom) can change their ordering. In solvents of high polarizability and/or at low temperature, state inversion may occur and S_1 acquires a nature

of B_u parentage. In fact, k_F at 77 K almost reaches the k_F^0 values calculated by the integrated absorption spectra (10^8 to 10^9 s⁻¹) pointing to an allowed character of the radiative transition.

The presence of the heteroatom affects also the photobehaviour of the thio-analogues of distyrylbenzene. Generally, the high emission yield of both the 1,4- and 1,3-substituted hydrocarbons is markedly reduced by the presence of the heteroatom, to an extent which depends on its position. The isomerization yield increases markedly for 1,3-di-(3'-thienylethenyl)benzene only (by almost one order of magnitude). The general effect is an increase in reactivity due to two factors: a less activated process in S₁ and an increase in the triplet population induced by the heteroatom.

In the study of the Z,Z and Z,E isomers of the distyrylbenzene analogues, the presence of adiabatic photoisomerization pathways (with direct formation of the excited E,E photoproduct) was nicely evidenced for some compounds by fluorimetry (in S₁) and by nanosecond laser flash photolysis (in T₁). However, the adiabatic mechanism was found to be poorly efficient if compared with the overall photoisomerization (that increases with respect to the hydrocarbon), pointing to a prevalent diabatic mechanism for the photoisomerization under direct irradiation. The mechanism changes from singlet adiabatic, in the case of 1,4-distyrylbenzene, to mixed singlet/triplet, adiabatic/diabatic, with a prevalent singlet diabatic contribution, in the case of the thio-analogues. As a matter of fact, the introduction of the sulphur heteroatom modifies the potential energy surfaces of S₁ lowering the energy barriers for rotation around the double bonds and stabilising the perpendicular configurations, thus favouring the diabatic pathways.

A different role is played by the sulphur heteroatom on the triplet reactivity of distyrylbenzenes. In this case, the sensitized E,E→Z,E quantum yield decreases, particularly when thiophene is the central ring, owing to fast adiabatic isomerization of Z,Z and Z,E towards the ³E,E* species (with quantum yields that, in some cases, reach the maximum value of 1 in the cis → trans direction in dilute solutions).

The results of measurements carried out with ultrafast spectroscopic techniques are in a general agreement with the fluorimetric results showing the formation of bands assigned to the S₁ → S_n transition decaying at a rate corresponding to the fluorescence lifetime. In one case, characterized by a substantial triplet yield, the formation of T₁ from the S₁ precursor and a role played by an upper S₂ state were also evidenced. Spectral changes observed in the 1-10 ps time domain were assigned to vibrational relaxations from hot vibronic levels or to solvent rearrangement.

Aza-derivatives

In these compounds, the position of the nitrogen atom in the side or central ring of distyrylbenzenes, the kind of conjugation (linear/crossed) and the solution pH are important factors in determining the relaxation pathways of the excited states. The behaviour of the neutral molecules in protic aqueous solvent was found similar to that in non-polar organic solvents whereas in acid medium the fluorescence quantum yield decreases by an order of magnitude for the protonated compounds, leading to high values of the photoreaction yield.

The presence of two main conformers, already observed in organic solvent for 2,6-distyrylpyridine and other cross-conjugated compounds, was also found in aqueous solutions, making the study more interesting but also more complicate.

The intermolecular interaction of these aza-compounds with the protic solvent breaks the intramolecular N-H interaction observed in non-protic solvent, particularly for the cross-conjugated compounds. Since this interaction has been reported to affect the conformational equilibrium (favouring the compressed rotamer) and to reduce the photoreactivity (which increases very little with respect to the hydrocarbon), the protic solvent allowed a substantial increase in the isomerization yield to be again observed and the position of the conformational equilibrium to be controlled.

An interesting effect was observed for 2,6-(phenylbutadienyl)pyridine, where the basic species leads to two isomeric photoproducts whereas the acid medium selectively produces the EZEE isomer having the cis bond adjacent to the central pyridine ring.

The present results offer a picture of the different behaviour of the neutral and protonated species and indicate the experimental conditions suitable to selectively induce a desired relaxation pathway.

Tatiana N. Orlova

Optical and spectral properties of liquid crystals with photosensitive chiral steroid dopant

Working place: Institute of Physics, National Academy of Sciences of Ukraine, Kyiv
Ph.D. Thesis 2007
Supervisor: Prof. Terenetskaya I.P.

Cis-trans isomerization is a ubiquitous photochemical process which forms the fundamental step in many photobiological processes, such as vitamin D synthesis, vision, phototaxis, etc. In last decade the influence of anisotropic liquid-crystalline (LC) microenvironment on the photoisomerization reactions of dopant molecules is the focus of interest in molecular photochemistry. On the other hand, the study of LC structure and optical properties changes as a result of phototransformations of photosensitive chiral dopants is one of the “hottest” areas in the liquid crystal physics today.

In this thesis the influence of UV-induced transformations of dopant chiral molecules 7-dehydrocholesterol (7-DHC, provitamin D₃) on the optical properties and structure of nematic and cholesteric LCs was investigated. At the same time, the features of previtamin D (photoisomer of 7-DHC) *cis-trans* photoisomerization in ordered LC media were studied using UV absorption spectroscopy.

It was shown, that interaction of steroid dopant molecules with host LC molecules affects both the 7-DHC absorption spectrum (bathochromic shift of 1.5nm) and the LCs transition temperature to isotropic phase (decrease of 0.5⁰C). These effects are enhanced under UV irradiation due to formation of flexible *trans*-isomer tachysterol.

Several new concentration and temperature effects on the efficiency of previtamin D *cis-trans* isomerization were observed in the LC matrices as compared to isotropic solvents [1, 2]:

1. at room temperature, in nematic LCs the efficiency of *cis-trans* isomerization increases significantly with raising of 7-DHC concentration (0.04 ÷ 3 wt.-%);
2. on the other hand, in induced cholesteric LCs (nematic + optically active dopant, OAD) the efficiency of *cis-trans* isomerization decreases with rising of OAD concentration from 1.6 wt.-% up to 60 wt.-%;
3. however, in highly twisted cholesteric LCs the minor rise of 7-DHC concentration (0.05÷2wt.-%) leads to remarkable increase of *cis-trans* isomerization efficiency similar to the case of nematic LC;
4. the above mentioned effects smoothed away with the temperature rising up to the point of complete disappearance in isotropic LC phase.

The numerical calculations showed that mere increase of individual previtamin D *cis-trans* isomerization quantum yield ϕ cannot explain the effects revealed. The value $\phi > 1$ defined from the spectral data led us to conclusion that previtamin D *cis-trans* isomerization in LC matrices acquired collective behavior with rising of 7-DHC concentration.

In the next chapter, the optical properties of nematic LC doped with 7-DHC were studied under UV irradiation using Stokes-polarimetry. It was found that contrary to initial 7-DHC with positive helical twisting power (HTP) $\beta_{7-DHC} = +3.5 \text{ mkm}^{-1}\text{wt.}\%^{-1}$, accumulated *trans*-isomer tachysterol was the left-handed chiral dopant with negative HTP $\beta_T = -8.5 \text{ mkm}^{-1}\text{wt.}\%^{-1}$ [3].

In addition, dynamics of cholesteric phase formation as a result of UV irradiation was studied, and significant differences in the dynamics were found depending on the ratio of initial cholesteric pitch value (the 7-DHC concentration) to the LC cell thickness:

1. in case of initial quasy-nematic phase (low 7-DHC concentration) small “islands” of planar-oriented left-handed cholesteric phase appeared at the beginning of UV irradiation and further these regions enlarged and merged with each other. Finally, left-handed cholesteric phase filled the whole LC cell volume. This process was identical in both “thin” ($d \approx 20 \text{ mkm}$) and “thick” ($d \approx 60 \text{ mkm}$) LC cells.

2. In case of initial right-handed cholesteric in “thick” LC cell ($d \approx 60 \text{ mkm}$), under UV irradiation the LC first re-oriented into homeotropic state (fingerprint texture was observed). Further planar-oriented left-handed cholesteric was formed. However, in case of “thin” LC cells ($d \approx 20 \text{ mkm}$) the fingerprint texture was not stable and arose simultaneously with planar-oriented regions.

In the last chapter effects of UV irradiation on the selective reflection of cholesteric LC's (nematic + OAD + 7-DHC) were studied in detail with the aim of monitoring the vitamin-D synthetic capacity of sunlight and/or artificial UV sources [4, 5]. The optimum LC composition which provided the largest shift of the selective reflection band ($\sim 150 \text{ nm}$) under UV irradiation was defined. Linear correlation of the shift with previtamin D accumulation in ethanol was established that formed basis for UV biosensor with visual estimation of previtamin D accumulation during an exposure [6].

The results obtained show promise of various applications such as UV dosimetry, optical information storage, LC display technology, etc.

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Renato Falcão Dantas***Ozonation of Emergent Contaminants***

Chemical Engineering Department, University of Barcelona, Spain

PhD thesis presented in July 5th of 2007.

Supervisors: Dr. Santiago Esplugas, Dr. Sandra Contreras

In this work, the ozonation of emergent contaminants represented by pharmaceuticals (Sulfamethoxazole and Bezafibrate) and surfactants (Quaternary Ammonium Compounds) was studied. Results in terms of target compound degradation and mineralization along with the biodegradability and toxicity assessment of formed intermediates are presented. Moreover, a previous study about the suitability of the combination ozonation-Sequencing Batch Biofilm Reactor (SBBR), using the model compound 4-chlorophenol, is shown.

The first part of this work deals with the removal and mineralization of the compound 4-chlorophenol. The 4-CP is not included among the “new” or emerging contaminants. However this preliminary study allowed setting up our ozonation system as well as analytical methods. In addition, the coupling ozonation with SBBR constitute an innovative experimental procedure.

The preliminary runs aimed to assess the mineralization of 100 and 200 mg L⁻¹ 4-chlorophenol (4-CP) solutions by ozonation and ozonation-biological treatment (SBBR). The experimental results showed that with an ozone flow rate of 5.44 and 7.57 g h⁻¹, 4-CP was completely removed from the solution in 15 and 30 minutes of ozonation, respectively. By the other hand, at the 4-CP abatement time, on average only 26 % of total organic carbon (TOC) removal was achieved. Quinone and hydroquinone were found as intermediates of reaction and a kinetic constant around 9·10⁻² min⁻¹ was calculated for the ozone direct attack. The biodegradability (BOD₅/COD) of the pre-ozonated solutions increased from 0 until a range between 0.2-0.37. The combination of ozonation and aerobic biological treatment in an aerobic sequencing batch biofilm reactor (SBBR) gave an abatement of more than 90 % of the initial TOC. Moreover, the biofilter reactor showed fast recuperation after being submitted to absence of oxygen and feed.

The Quaternary Ammonium Compounds (QACs) ozonation was carried out in order to assess the mineralization potential of ozonation processes for this class of compounds. To perform this study, the QACs 16-BAC (Benzyl-dimethyl-hexadecylammonium-chloride) and 18-BAC (Benzyl-dimethyl-stearylammmonium-chloride) were treated by ozonation at different O₃ dosage. The TOC (Total Organic Carbon) removal was monitored in order to follow the mineralization of the surfactants along the runs. According to experimental results, from an initial TOC concentration of 50 mg L⁻¹, 90 minutes of ozonation reached at most 50% of mineralization at the used conditions (ozone flow rate 7.57 g h⁻¹). Due to the experimental problems observed during the ozonation of QACs, an alternative advanced oxidation process (photo-Fenton) was applied. In order to observe the mineralization of QACs by means of photo-

Fenton, the runs were carried out with the same QAC concentration used in ozonation runs. Besides, two different lamps were used (UV and Xe). According to experimental results, after 90 minutes of treatment, the photo-Fenton process achieved up to 80% of mineralization when the UV lamp was used. The efficiency of the photo-Fenton with Xe lamp was lower. An overall view of the two used oxidation process allows to state that the photo-Fenton process seems to be the most suitable process to treat waters containing QACs.

To carry out the study of the sulfamethoxazole (SMX) ozonation, 200 mg L⁻¹ SMX solutions were treated by ozonation at different pH. Results showed that ozonation was proved to be an efficient method to degrade sulfamethoxazole. After 15 minutes of ozonation (corresponding dose = 0.4 g of ozone L⁻¹), the complete antibiotic abatement was almost achieved with just 10 % of mineralization. The biodegradability and toxicity of the ozonation intermediates were also studied. A biodegradability enhancement (increment of BOD₅/COD ratio) from 0 to 0.28 was observed after 60 min of ozonation. The acute toxicity of the intermediates was followed by the Microtox[®] test and the toxicity profile showed a slight acute toxicity increment in the first stage of ozonation. The pH variation had an important role in the TOC and COD removal, promoting their growth with the increment of alkalinity. The second order kinetic constants for the ozonation of the SMX in an order of magnitude of 10⁵ L mol⁻¹ s⁻¹ were also determined for pH 5 and 7.

Concerning the Bezafibrate (BZF) ozonation, the results showed that ozonation is an efficient method to degrade BZF: after 10 minutes of treatment (corresponding to a dose of 0.73 mmol L⁻¹ of ozone), the complete BZF abatement is achieved, starting from an initial concentration of 0.5 mmol L⁻¹. However, only a small part of the substrate is mineralized. Two different experimental approaches (absolute and competition method) are adopted to estimate the second order kinetic constants for the ozone attack at pH=6.0, 7.0 and 8.0. A good agreement was observed between the two kinetic methods adopted. The identification of main intermediates, attempted by HPLC-MS technique, indicates that the oxidation of BZF develops through both the hydroxylation of the aromatic ring and the attack of ozone on the unchlorinated aromatic one. The assessment of by-products biodegradability and acute toxicity demonstrates that ozonation is a suitable technique to improve the biodegradability and reduce the toxicity of waters containing BZF.

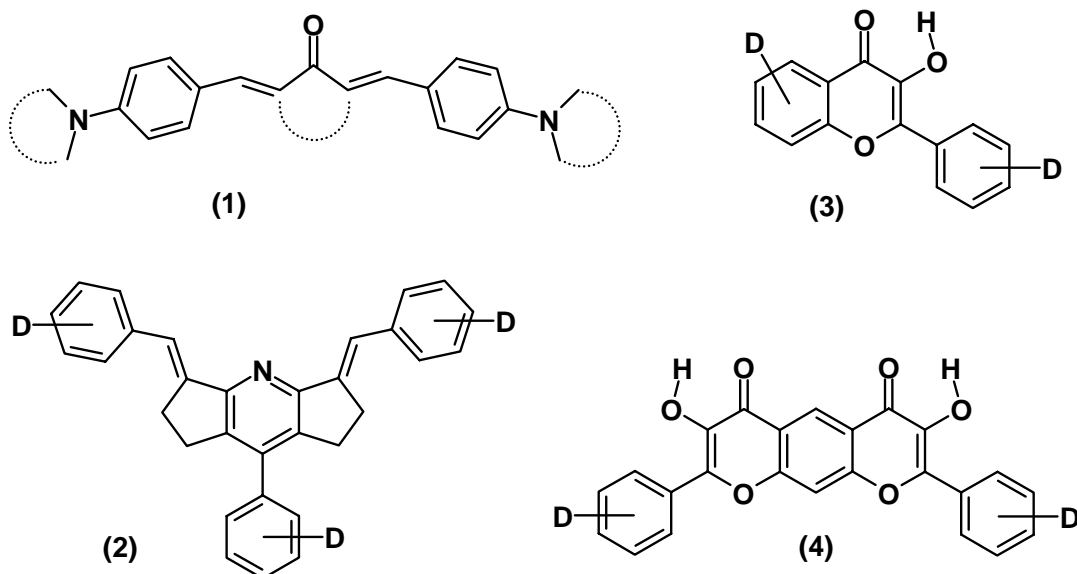
Vasyl G. Pivovarenko

Synthesis, structure and properties of multi-channel fluorescence probes on the basis of 1,3-diarylidene ketones, dicyclopenta[b,e]pyridines and 3-hydroxychromones

Chemistry Faculty, National Taras Shevchenko University of Kyiv, Ukraine
Thesis of D. Sci. on organic chemistry (in Ukrainian), September, 2007

Development of multi-channel fluorescence probes on the basis of mentioned in the title classes of dyes was implemented. Multi-channel fluorescence probes report about the events in studied

object by several channels, each presented by separate region of excitation or emission spectrum of the probe. This allows to collect the most precise and detailed information about the object. Ratiometric probes present the devices with two informational channels.



D: electron donor substituent with a function of linker, receptor of analyte, etc.

After the consideration of probe constitution and mechanisms of probe functioning two of the most prospective mechanisms – an intramolecular charge transfer (ICT) and excited state intramolecular proton transfer (ESIPT) were used in the probe design. The series of new fluorescence probes (1) from 1,3-diarylidene-cyclopentanones, diarylideneacetones and diarylidene-cyclohexanones were synthesized. High efficiency of bis-crown derivatives in the recognition of Ba^{2+} and Mg^{2+} cations as well as high resolution (7000 cm^{-1}) of fluorescence bands of the ligand and magnesium complex was registered for them. Diarylidene-cyclopentanones were applied in the study of hydrogen bonding interactions with proton donor molecules and for the study of polarity of separate sites of lipid membranes.

A new group of fluorescence dyes from 3,5-diarylidene-dicyclopenta[*b,e*]-pyridines (2) was synthesized. The properties of their representatives were studied. It was shown that these dyes have high (30-70%) fluorescence quantum yields, displaying the emission in blue, green, yellow and red regions of spectrum. A series of ratiometric fluorescence pH indicators was synthesized for the measurements of pH in the range from 2 to 11.

A series (3) of 3-hydroxychromone (3HC) derivatives of designed structure were synthesized. There were obtained the dyes containing substituents of different π -donating ability, or with different planarity of the molecule as well as with different chromophore length, or with increased chromophore rigidity. The correlations in the structure of dye molecule and the positions of absorption and emission bands, as well as the two emission bands intensity ratio, or the fluorescence quantum yield were estimated and discussed. The dependences of mentioned properties upon the solvent parameters were estimated. The synthesized dyes were applied in the study of the properties of homogeneous and microheterogeneous liquids, including cell organelles. A method of fluorometric determination of hydrogen bond donor component in two-component homogeneous liquid together with polarity parameter as a function of dielectric constant was proposed. The 3HC probes were applied in the study of physical processes in lipid membranes, where their considerable advantages were displayed in comparison with the probes

of other types. The probe with high sensitivity to non-specific interactions and no response to hydrogen bond donors in solutions was synthesized and studied. A wide-range fluorescent pH indicator on the basis of 3,4'-dihydroxyflavone was developed and studied, as well as the probe for determination of adenosine triphosphate in aqueous solutions, in its physiological range of concentrations.

The representatives of diflavonols (4) – a new class of dyes were synthesized, and their fluorescence properties were studied. Due to the presence of two ESIPT systems in the molecule the dyes can display single and double proton transfer phenomena giving three tautomeric forms (NN*, NT* and TT*) in S_1 state. Theoretical methods were applied in the study of structure, including the possibilities of synchronous and consecutive processes of intramolecular double proton transfer in diflavonols. It was estimated that diflavonols have unique fluorescence properties, such as two- and three-band emission, high (50-60%) quantum yields, record sensitivity to polarity and hydrogen bond donor ability of surroundings, high Stokes shifts (6500-10000 cm^{-1}) and fluorescence in wide region of spectrum (450-650 nm).

Books

Principles and Applications of Fluorescence Spectroscopy

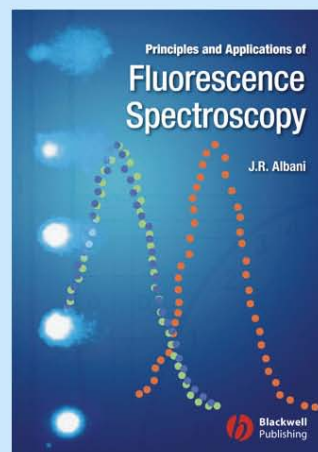
OUT NOW...

Physical
ChemistryPrinciples and Applications of
Fluorescence Spectroscopy**JIHAD RENE ALBANI**

University of Lille

Fluorescence spectroscopy is an important investigational tool in many areas of analytical science, due to its extremely high sensitivity and selectivity. With many uses across a broad range of chemical, biochemical and medical research, it has become an essential investigational technique allowing detailed, real-time observation of the structure and dynamics of intact biological systems with extremely high resolution. It is particularly heavily used in the pharmaceutical industry where it has almost completely replaced radiochemical labelling.

Principles and Applications of Fluorescence Spectroscopy gives the student and new user the essential information to help them to understand and use the technique confidently in their research. By integrating the treatment of absorption and fluorescence, the student is shown how fluorescence phenomena arise and how these can be used to probe a range of analytical problems. A key element of the book is the inclusion of practical laboratory experiments that illustrate the fundamental points and applications of the technique.



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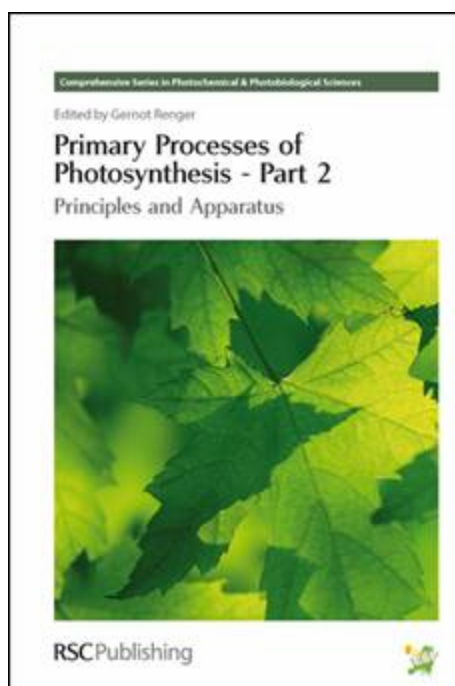
BOOKS

Primary Processes of Photosynthesis

RSC Book Publishing is very excited to announce the publication of **Primary Processes of Photosynthesis**, the two volume, major reference work by Gernot Renger.

Primary Processes of Photosynthesis have been researched and analysed for generations and in this two part set the Editor has brought together contributions from numerous leading scientific experts providing a compendium of information offering the most up-to-date understanding of the primary processes of photosynthesis.

This outstanding work represents the activity of researchers across the globe and will be of utmost interest to all those working in the fields of Photochemistry, Bio-organic Chemistry, Bio-inorganic Chemistry, Crystallography, Biological Sciences, Biochemistry and related disciplines.



CONFERENCE REPORTS

XXIIIrd International Conference on Photochemistry (ICP 2007) July 29– August 3, 2007, Cologne, Germany

The XXIIIrd International Conference on Photochemistry was held in Cologne / Köln from July 29 until August 3, 2007. This congress was organized by an international committee chaired by Ken Ghiggino from Australia and a local committee chaired by Axel Griesbeck from Cologne. Co-organization came from the German Chemical Society (GDCh Photochemistry Subgroup) and the German Bunsen Society for Physical Chemistry (DBG). The local organization was assisted by Klaus Meerholz (Physical Chemistry, University Cologne), Klaus Warzecha (Max-Planck-Institute for Bioinorganic Chemistry) and Axel Klein (Inorganic Chemistry, University Cologne). We had 547 participants from 46 countries presenting 125 oral contributions in three parallel sessions and 400 poster contributions.

Robert Huber (Martinsried, Germany), Nobel laureate in chemistry 1988, described in the opening keynote lecture that protein crystallography experienced in the last twenty years a rapid development in methods and instrumentation, allowing the determination of very large and complex protein structures, particularly when combined with electron microscopy. These structures are the basis for understanding their binding specificities and catalytic properties, their spectral and electron transfer properties and their roles in physiological systems, thus combining aspects of chemistry, biology, physics, and medicine, and allowing the design and development of specific ligands of target proteins opening novel ways for therapeutic intervention and for plant protection.

Ken Ghiggino (Melbourne, Australia) gave a plenary talk on electron and energy transfer dynamics and described the way from simple models to macromolecules. Understanding and optimizing photoinduced energy and electron transfer processes continues to provide major challenges for photochemists. These processes often precede photodecomposition and underpin the operation of photosynthetic mimics, solar cells and molecular electronic devices. In his presentation he reviewed advances in our understanding of energy and electron transfer processes in model chromophores, supramolecular assemblies and macromolecules.

Karl Leo (Dresden, Germany) discussed in his keynote lecture the recent progress in the field of organic LED including results on OLED with doped transport layers. Organic materials can be efficiently doped, enabling significantly improved devices due to the high conductivity of transport layers and due to improved injection at the contacts. Additionally, a novel approach to efficient white OLED was reported: by a suitable management of singlet and triplet excitons, it is possible to realize white OLED having nearly 100% internal quantum efficiency without using blue phosphorescent emitters, thus circumventing the stability problems of these emitters.

Jürgen Troe (Göttingen, Germany) reported on the photochemistry of aldehydes and named his plenary lecture “A New Twist on an Old Subject”. He could show that the photochemistry of simple aldehydes which is of importance for atmospheric chemistry, is intimately related to the chemistry which is observed during pyrolysis in combustion processes. Photoactivation in the near UV through internal conversion produces the same vibrationally highly excited ground state molecules as does collisional activation in hot gases. A theoretical description was presented that combined dynamical and statistical, classical and quantum elements. The

photochemistry of larger aldehydes was reviewed in the light of the new picture of formaldehyde photochemistry.

Abderrazzak Douhal (Toledo, Spain) gave a plenary lecture on the femtosecond dynamics of pharmaceutically active molecules in solution. He described fast and ultrafast events of selected medicines in solution and in cyclodextrins. His results demonstrated that H-bonding and confinement of the environment affect the relaxation dynamics and the nature of the resulting products. The dynamic studies were performed in the time regime of 100 fs to 10 ps and resulted in a better understanding of piroxicam, a [non-steroidal anti-inflammatory drug](#) and related medicines. Professor Douhal will be the local organizer of the next ICP conference in Toledo in 2009 and presented first-hand information on this location.

The first monday **Session 1** on single molecule spectroscopy was opened by an invited lecture by **Christoph Bräuchle** (Munich, Germany) on single molecules in nano- and biosystems. The detection of single fluorescent molecules and their dynamics in nanoporous systems as well as biological applications such as the analysis of infection pathways of a single virus in a living cell were reported. The following talks comprised perylene diimide dendrimers as single photon source (Michel Sliwa, Leuven) and single molecule spectroscopy of conjugated polymers (Manfred Walter, Salt Lake City).

Session 2 was devoted to special effects in high intensity laser fields. **Nobuaki Nakashima** (Osaka, Japan) spoke about non-linear phenomena during the excitation of molecules by intense femtosecond pulses, i.e. the formation of intact molecular ions and multiphoton absorption in solution. The formation of triatomic hydrogen molecule cations from ultrashort intense laser photolysis of methanol was reported by **Kaoru Yamanouchi** (Tokyo, Japan). He could show that hydrogen migration from C to O proceeds faster than the pulse duration of 7 fs. Syoji Ito (Osaka, Japan) reported on the local temperature at the focus of near IR laser beams in optical tweezing experiments determined by fluorescence correlation spectroscopy.

Session 3 focussed on chirality effects in photochemistry and was opened by an invited lecture by **Anne Zehnacker-Rentien** (Paris, France) on jet-cooled hydrogen-bonded complexes of chiral molecules studied by fluorescence and IR spectroscopy. These studies revealed the importance of weak non-covalent binding motifs in chiral recognition. The other contributions were presented by Cheng Yang (Osaka, Japan) on supramolecular photochirogenesis with cyclodextrins and cucubiturils and by Rudolf Pietschnig (Graz, Austria) on MLCT and configurational photoisomerization in ferrocenyldiphosphenes.

Session 4 on theoretical photochemistry was opened by an invited lecture by **Massimo Olivucci** (Siena, Italy) on ab initio multiconfigurational quantum chemistry in photobiology. He reported on a hybrid quantum mechanics / molecular mechanics computational strategy based on MC perturbation and CAS-SCF geometry optimization applied for static and dynamic investigation on rhodopsin proteins and the green fluorescent protein. Bernhard Dick (Regensburg, Germany) described the localization of conical intersections relevant for photochemical reactions, Lluís Blancafort (Girona, Spain) theoretical studies of reactive and degradative excited-state properties of DNA nucleobases. Christel Marian (Düsseldorf, Germany) showed the importance of spin-orbit coupling parameters for photobiologically relevant molecules, Jacek Waluk (Warsaw, Poland) reported on the mechanistic aspects of single and multiple proton / hydrogen transfer in porphyrins and porphycenes. Luis Frutos (Madrid, Spain) showed the role of stretching modes in nonvertical triplet-triplet energy transfer in trans-stilbene, and Gerrit Groenhof (Göttingen, Germany) described CASSCF / force field calculations on photoreceptor proteins and DNA excited state decay.

Femto(bio)chemistry was the topic of **Session 5** which was started with an invited lecture by **Nikolaus Ernstring** (Berlin, Germany) on femtosecond solvation dynamics in DNA double helices. By studying time-dependent solvation it is possible to record the dielectric dispersion

and the local polarity in a DNA environment. Additional talks were presented by Satoshi Habuchi (Boston, USA) on a single molecule view of eukaryotic DNA replication initiation, Tomoyuki Yatsushashi (Osaka, Japan) on the direct desorption ionization of organic molecules in solid state by intense femtosecond laser pulses, Dimitra Markovitsi (Gif-sur-Yvette, France) on DNA double helix fluorescence studied by femtosecond spectroscopy, Melinda Noronha (Lisbon, Portugal) on the tracking of local conformational changes of ribonuclease A using time-resolved fluorescence and by Satoshi Takeuchi (Hiroshima, Japan) on real-time probing of structural dynamics in cis-stilbene photoisomerization by ultrafast Raman spectroscopy.

Session 6 on charge transport was the last Monday session and started with an invited lecture by **Murthy Gudipati** (Pasadena, USA) on organic photochemistry in cryogenic ice matrices. He described the ionization of organic polyaromatics in ice matrices as a new photochemical channel leading to long-term stabilized radical cations with consequences for astrophysical and atmospheric phenomena. Wolfgang Seitz (Erlangen, Germany) described the synthesis and properties of bio-inspired electron donor-acceptor hybrids, Hans-Christian Becker (Uppsala, Sweden) the bridge-mediated photoinduced electron transfer in strongly coupled zinc-gold porphyrine dyads. Through bond electron exchange in ethynyl-naphthalene-based molecular bridges was reported by Andrew Benniston (Newcastle, UK), electron transfer reactions in designed donor-bridge-acceptor systems by Bo Albinsson (Göteborg, Sweden). Christoph Lambert (Würzburg, Germany) analyzed electron transfer properties in mixed valence compounds by Jortners theory and Günther Knör (Linz, Austria) gave insight into electronic transitions and the photochemistry of novel organometallic multichromophoric complexes.

The first Tuesday **session 7** was devoted to aspects of applied photochemistry and started with an invited lecture by **Luisa De Cola** (Münster, Germany) titled “assembling photoresponsive molecules, nano-objects, and living systems”. She illustrated how nano-objects, in particular zeolithe L can be assembled and non-covalently linked to living objects. Zeolithes, filled with fluorescent dyes can be used to monitor the motion of bacteria and to observe cellular uptake mechanisms. Other talks were presented by Bernd Strehmel (Osterode, Germany) on the rapid change in printing industry from conventional lithography to high-speed laser systems and Adam Moulé (Cologne, Germany) on light intensity dependent charge recombination at the anode in bulk-heterojunction solar cells. Hartmut Yersin (Regensburg, Germany) described the basic emission properties of triplet emitters applied in organic light-emitting diodes.

Session 8 on photoinduced electron transfer (PET) processes began with an invited talk by **Jye-Shane Yang** (Taipei, Taiwan), who described aminostilbenes as molecular probes for the study of twisting processes in photoinduced intramolecular charge transfer (ICT) states. For these substrates, the famous TICT state was concluded to be unimportant in excited state decay. Eric Vauthey (Geneva, Switzerland) reported an experimental study of the interplay between photoinduced electron transfer and reorientational motion, Stephan Landgraf (Graz, Austria) described Rehm-Weller and Stern-Volmer experiments in the light of remote electron transfer. The mechanism of contact and remote electron transfer was finally discussed on theoretical grounds by Anatoly Burshtein (Rehovot, Israel).

Session 9 on photocatalysis was opened by an invited talk by **Tetsuro Majima** (Osaka, Japan), who by studying the one-electron of aromatic compounds during the photolysis of TiO₂ particles by time-resolved laser spectroscopy, gained more insight into the mechanisms of semiconductor photocatalysis. Johan Hofkens (Leuven, Belgium) showed how single molecule fluorescence microscopy allows the study of heterogeneous catalysis, Martin Demuth (Mülheim, Germany) described the generation of hydrogen and oxygen from water and titanium disilicide as photocatalyst and solar irradiation. Sven Rau (Jena, Germany) showed that photocatalytic hydrogen production is possible using oligonuclear ruthenium complexes.

Aspects of basic photochemistry were the topic of **Session 10**. **Jörn Manz** (Berlin, Germany) reported in an invited lecture on quantum dynamics simulations which were used to predict photochemical processes initiated by ultrashort attosecond laser pulse excitation such as the control of electric ring currents in oriented molecules by circularly polarized laser pulses. Femtosecond laser pulse initiated processes were also described by Søren Rud Keiding (Aarhus, Denmark) for the photolysis of formide and by Jörg Schröder (Göttingen, Germany) for the photoinduced decomposition of aryl peroxy carbonates. Alexey Baklanov (Novosibirsk, Russia) described the photochemistry of van der Waals complexes of molecular oxygen with organic molecules, Elena Ishow (Cachan, France) the reversible holographic fluorescent patterning through photoinduced mass migration in photoactive monomers. Franklin Vargas (Caracas, Venezuela) described in vitro studies of photooxidative properties of new quinolone antibiotics by chemiluminescence assay, and Nobuhiro Ohta (Sapporo, Japan) the remarkable temperature dependence of external electric field effects on photochemical reactions.

An invited lecture by **Simone Techert** (Göttingen, Germany) started **Session 11** on photophysical techniques. She spoke on current studies of subpicosecond time-resolved X-ray diffraction / scattering experiments on chromophoric systems for the structural analysis of ultrafast dynamic processes. Masahide Terazima (Osaka, Japan) reported on spectroscopically silent photosensor molecules analyzed by the laser-induced transient grating method, Silvia Braslavsky (Mülheim, Germany) explained that a large entropic term due to water rearrangement is concomitant with the photoproduction of anionic free-base porphyrin triplet state in aqueous media. Claire Niezborala (Palaiseau, France) described the application of time-resolved circular dichroism in the far UV for the study of conformational changes in proteins, Anna Diller (Leiden, Netherlands) the use of photo-CIDNP MAS NMR analysis for the investigation of the origin of the high redox force of photosystem II. The nonadiabatic coupling mechanism for ultrafast electron transfer in bacterial reaction centers was reported by Sighart Fischer (Garching, Germany), and Eberhard Riedle (München, Germany) described dynamics in naphthalene bisimides designed for optoelectronic applications.

The fascinating world of quantum dots was the topic of **Session 12**. In an invited lecture, **Ya-Ping Su** (Clemson, USA) analyzed the photoluminescence properties of small carbon nanoparticles with sizes less than 10 nm. These quantum dots may find applications beyond those of traditional semiconductor QD, e.g. in binding biologically active molecules when appropriately derivatized. Corola Krysch (Erlangen, Germany) spoke on a femtosecond study of ultrafast exciton dynamics in silicon QD, Eduard Zenkevich (Minsk, Belarus) described relaxation processes in nanocomposites based on CdSe/ZnS nanocrystals and porphyrine molecules. Bronislaw Marciniak (Poznan, Poland) explained the effects of solvent and salts on the photochemical oxidation of phenylthioacetic acid, Hirendra N. Ghosh (Mumbai, India) the effect of size quantification of TiO₂ QD on interfacial electron transfer dynamics. Nanoscale resolution was described by Hiroshi Fukumura (Sendai, Japan) for photoluminescence and Raman scattering of nanostructures under scanning tunnelling microscopy, and Vladimir Razumov (Moscow, Russia) talked on the synthesis and optical properties of fluorescent colloidal QD in reverse micelles.

In appreciation of their significant contributions to the field of photochemistry and photophysics, two young scientists, Manuela Schiek and Anton Granzhan, were honoured with the **Albert-Weller Prize 2007** during the Wednesday morning session. In the course of her Ph. D. thesis **Dr. Manuela Schiek** (Oldenburg, Germany) has developed a route to grow a new type of light emitting devices consisting of functionalised organic molecules forming organic nanofibres via molecular self assembly. As compared to their inorganic counterparts these aggregates exhibit extraordinary optoelectronic flexibility and brilliant performance which makes them attractive for incorporation into radically new optoelectronic devices also in view

of their particular morphology. Anisotropic luminescence, waveguiding, non linear optical response, random lasing, electrical mobility and mechanical stability are some of the outstanding properties of this new class of materials. In order to optimise the molecular building blocks for most efficient photon upconversion to allow even non-linear microscopy of single nanofibres Dr. Schiek has not only used modern methods in physics and physical chemistry but has also developed new routes in high end organic synthesis on equal footing. In his interdisciplinary and highly demanding studies, **Dr. Anton Granzhan** (Siegen, Germany) synthesized and investigated three different groups of functional organic dyes that were designed to be applied as DNA-sensitive fluorescent light-up probes, as triplex-DNA binders, and as selective guest molecules for DNA hosts with abasic positions. With talent, creativity, and extraordinary synthetic and analytical skills, he employed photochemical and photophysical methods efficiently to assess the mode of action of a series of fluorescent probes and to gain more insight into the interplay between organic ligands and biomacromolecules. Overall, Dr. Granzhan presented an important contribution to modern organic photochemistry, and he demonstrated the significant impact of photochemical tools on interdisciplinary research at the borderline to materials science and bioorganic and medicinal chemistry.

In appreciation of his significant contributions to the field of photochemistry and photophysics, **Professor Gion Calzaferri**, University Berne, was honoured with the **Theodor Förster prize 2007**. This award honours his pioneering work in which he links aspects of organic photophysics with inorganic chemistry to hybrid systems with unique properties. His work on energy and electron transfer of organic dye molecules in zeolites is highly fundamental and belongs to the most accurately performed investigations in this area. His research stands in a direct scientific tradition to the work by Theodor Förster on the radiationless resonant transfer of electronic excitation energy from donor to acceptor molecules. Gion Calzaferri is a scientist of high originality and creativity. In his research lifework he has focussed on the elucidation of photochemical and photophysical problems and recently also in the application of photochemical processes for the environmentally save utilization of solar energy.

Chemiluminescence and reactive oxygen were the topics of **Session 13**, introduced by an invited lecture by **Michael Orfanopoulos** (Heraklion, Greece). He described the current controversial concepts of the singlet oxygen photooxygenation of olefins and showed special designed molecular probes for the investigation of these mechanisms. Further talks were presented by Torsten Linker (Potsdam, Germany) on singlet oxygen as a tool for lithography and molecular motors, Wilhelm Baader (São Paulo, Brasil) on the excited state generation in cyclic peroxide decomposition, Alexey Trofimov (Moscow, Russia) on the excited-state generation as an experimental tool for studying oxidative and antioxidative processes, Leticia González (Berlin, Germany) on the dual photochemistry of anthracene-9,10- endoperoxide, and Helmut Görner (Mülheim, Germany) on the oxygen uptake via triplet quenching of quinones by formate, ascorbate, and alcohols.

Session 14 was on polymers and photochemistry and started with an invited lecture by **Irene Burghardt** (Paris, France) on the photophysics of π -conjugated organic semiconductor systems. A non-adiabatic quantum dynamics based on a hierarchical electron-phonon model was presented to rationalize ultrafast exciton dissociation in these semiconductor polymers. Tatsuya Fujino (Tokyo, Japan) described ultrafast solvation dynamics of hydrophilic polymer particles, Jürgen Stumpe (Potsdam, Germany) the photoorientation of ionic azobenzene-surfactant self-assembly complexes, and Martin Vacha (Tokyo, Japan) conformational and photophysical properties of single conjugated polymer molecules studied via their absorption ellipsoids. Yi Li (Beijing, China) gave a talk on the intramolecular electron transfer and exciplex formation as probe to detect the folding back conformation of poly(arylether)

dendrimers, and Nikolai Petrov (Moscow, Russia) on the nano-sized structure effect on the cyanine-dye relaxation from electronically excited states in binary liquid mixtures.

Session 15 had photoactive biomolecules as topic and started with an invited talk by **Pascale Chagnenet-Barret** (Paris, France) on the role of the chromophore photophysics and of the local environment on the primary steps of the photoactive yellow protein (PYP) photocycle. She reviewed the role of both the intrinsic photophysics of the chromophore and the local environment on the short-time dynamics of the PYP photocycle by subpicosecond transient absorption spectroscopy. Marius Schmidt (Garching, Germany) reported on cis/trans isomerizations in photoactive proteins investigated by (time-resolved) X-ray crystallography, Kyril Solntsev (Atlanta, USA) on the meta and para effects in the photophysics of the green fluorescence protein chromophores, and Tilman Kottke (Bielefeld, Germany) on the photoactivation of the sensory blue light receptor cryptochrome from *Arabidopsis* and *Drosophila*. Craig Lincoln (Melbourne, Australia) spoke on the development of a high signal-to-noise UV confocal microscope for multi-photon imaging of endogenous fluorescence, Marina Kuimova (London, UK) on porphyrin oligomers for photodynamic therapy via two-photon excitation.

Session 16 on singlet oxygen was dedicated to Waldemar Adam on occasion of his 70 birthday and was composed of several invited talks and oral communications: **Eva Hideg** (Szeged, Hungary) gave a presentation on special reactive oxygen species indicator reagents for detecting singlet oxygen in plants, Chen-Ho Tung (Beijing, China) on nano-space as found in microreactors to control selectivity in the photooxygenation of alkenes, **Santi Nonell** (Barcelona, Spain) talked on porphycenes, compounds with new chemistry and one- and two-photon photosensitising properties for application in photodynamic therapy, Kamil Lang (Řež, Czech Republic) described new materials producing singlet oxygen, **Robert Redmond** (Boston, USA) spoke on the effect of sub-cellular localization of singlet oxygen reactions and subsequent distant effects through secondary oxidative processes in cell populations, Kazutaka Hirakawa (Hamamatsu, Japan) described the photosensitized singlet oxygen generation in the microenvironment of DNA strands, and **Peter Ogilby** (Aarhus /Denmark) explained experiments with sub-cellular resolution in single cells using his singlet oxygen microscope.

Session 17 on spectroscopic methods and applications started with an invited lecture by **Claus Seidel** (Düsseldorf, Germany) on molecular Ångström optics. He described the use of multiparameter fluorescence detection for studies on biological systems labelled with a fluorescent donor and acceptor dye performing single-molecule fluorescence resonance energy transfer (FRET). Werner Fuss (Garching, Germany) described dark intermediate states in pericyclic photochemical reactions, detected by ultrafast spectroscopy, Ortwin Brede (Leipzig, Germany) femtosecond events in bimolecular free electron transfer processes, and Tatiana Nikipelova (Moscow, Russia) the use of photochemical reactions as reflection of the microstructure of solvent mixtures. Nina P. Gritsan (Novosibirsk, Russia) described a study of ultrafast hydrogen atom and acyl group transfer by transient absorption spectroscopy and computational chemistry, Antony Harriman (Newcastle, UK) spoke on light harvesting and subsequent charge separation in borondipyrromethene (BODIPY) based arrays, and Sophie Badré (Cachan, France) described the solid-state fluorescence of new Bodipy derivatives as tool for the development of molecular nanosensors.

Session 18 had energy transfer processes in its focus and was opened by an invited lecture by **Trevor Smith** (Melbourne, Australia) on time-resolved total internal reflection fluorescence studies of macromolecular absorption. Complex time-dependent fluorescence anisotropy data and its interpretation in terms of rotational motion, excited-state dynamics and macromolecular conformation were reported. Olga Fedorova (Moscow, Russia) described structure and molecular properties of assemblies of heterostilbene molecules, Werner Nau (Bremen, Germany) presented self-assembling supramolecular metalloenzyme models

displaying photocatalytic activity, and Xavier Allonas (Mulhouse, France) described an experimental and computational study of 2-Hydroxy-2,2-dimethylacetophenone photodissociation. Galina Loukova (Chernogolovka, Russia) spoke on a study of triplet-triplet energy transfer and coordination between d^0 metallocenes (Zr, Hf) and unsaturated hydrocarbons, Albert Brouwer (Amsterdam, Netherlands) on mechanistic studies of light-activated translational motors, and Hiroshi Masuhara (Osaka, Japan) presented a mechanistic study of femtosecond laser-induced crystallization.

Aspects of water dynamics were summarized in **Session 19**. **Thomas Elsässer** (Berlin, Germany) reported in an invited lecture on hydrogen bonded dimers in liquids. Ultrafast nuclear motion, vibrational couplings and dissipation for two model compounds, the cyclic acetic acid dimer and the dimer of 7-azaindole were described. Damien Laage (Paris, France) presented results of the reorientational dynamics of water molecules in anionic hydration shells, Peter Vöhringer (Bonn, Germany) spoke on vibrational energy relaxation versus spectral diffusion studied by femtosecond mid-infrared spectroscopy on liquid-to-supercritical water, Keitaro Yoshihara (Nagakute, Japan) reported the UV-light-induced water-droplet formation from wet ambient air. Ehud Pines (Beer-Sheva, Israel) described base-induced solvent switches in acid-base reactions.

Session 20 on photocages and photoprotection started with an invited lecture by **Peter Ford** (Santa Barbara, USA) on polychromophoric compounds for the photogeneration of bioactive agents. A number of potential NO precursors like nitrito complexes of Mn and Cr as well as QD with dye ligands were reported. Wen-Sheng Chung (Hsinchu, Taiwan) described the Cu(II)-triggered fluorescence on-off/off-on switchable calix[4]arene chemosensors, Petr Klán (Brno, Czech Republic) synthetic and mechanistic variations of the photoenolization reaction. Alberto Soldevilla (Köln, Germany) presented the chiral 3-(2-phthalimido-propionate)yl photocages for the carboxylate group based on a photoinduced electron transfer process, and Peter Gilch (München, Germany) reported on femtosecond studies of the hydrogen transfer in nitroarenes.

The final **Session 21** was entitled environmental photochemistry. In an invited lecture, **Silvio Canonica** (Dübendorf, Switzerland) gave an overview on electron transfer to excited triplet states as a relevant process in aquatic photochemistry, e.g. for water purification and disinfection. Irina Sokolova (Tomsk, Russia) described the fluorescence analysis of sequential UV-biological degradation of cresols in water and in humic water, Kazuhiko Shibuya (Tokyo, Japan) the photochemistry of ozone-water complex in cryogenic matrices, Emma Coyle (Dublin, Ireland) spoke on solar photooxygenations as a “green route” to quinonoid fine chemicals, and Alex Orlov (Cambridge, UK) on doped and nanoparticle modified semiconductors for environmental photocatalysis.

The future of photochemistry is bright. This impression is inescapable when one recapitulates the topics of the conference. The discipline becomes more and more biological and material oriented, more physical and more applied. This makes discussions between photochemists sometimes complicated but fascinating, considering the difference in special languages and the range of subdisciplines.

Axel Griesbeck (Cologne)

CONFERENCE REPORTS

4th Joint Meeting of Photobiology and Photochemistry “PhotoBioChem ‘07” June 6-9, 2007, Acquafredda di Maratea, Italy,

The fourth Joint Meeting of the Italian Photobiology Society (SIF) and the Italian Group of Photochemistry (GIF) took place successfully on June 6-9, 2007 in Acquafredda di Maratea, a magnificent site on the Tyrrhenian coast of the Basilicata region, very close to the place where the second Joint Meeting was done in 1996. The format of the previous meetings was repeated starting each session with invited lectures dealing with topics of general interest, for plenary audience, and followed by parallel sessions devoted to short oral communications and poster presentations, specifically dedicated to photochemists and photobiologists, respectively.

Three plenary and four key lectures were given. Santi Nonell (Barcelona) provided an overview on the technical progress and new insights for time-resolved singlet oxygen detection in biological systems. Nicola Armaroli (Bologna) illustrated the actual state of the energy request and the future perspectives pointing the attention on challenges and opportunities for humanity and science. Cristiano Viappiani (Parma) discussed the acid unfolding and proton transfer equilibria in proteins studied by laser pH-jump methods. Maurizio Fagnoni (Pavia) talked about the effect of trimethyl-silyl group on the production and reactivity of phenylium cation. Antonino Mazzaglia (Messina) reported on the connection between structural properties and functionality in nano-aggregates between cyclodextrin (carrier) and porphyrin (photosensitizer). Massimo Trotta (Bari) discussed environmental modulation of the energetics in the photosynthetic reaction centre from purple bacteria. Salvatore Sortino (Catania) gave an overview on nano-assembled systems able to photorelease nitric oxide.

The 41 oral and 31 poster presentations covered a wide range of the scientific activity developed by the two associations. Several contributions from photochemists were devoted to photoprocesses in supramolecular species, photochemistry of various nanoparticles, new types of photochromic systems, drugs interaction with DNA, theoretical study of photochemical processes and photochemistry of natural products. The main topic treated by photobiologists concerned the effect of light on the photoreceptor systems of plants and microorganisms, studied by the behavioural or genetic point of view. Two communications treated the autofluorescence of tissues and its relevance in terms of early diagnosis of diseases. Other contributions dealt with photostability of drugs and photosensitization by porphyrins and other compounds, stressing the possible new applications in terms of decontamination of polluted water and anticancer therapy.

The number of participants was about 100, among them a large number of young researchers who distinguished themselves in brilliant presentations of their research work. The crowded scientific programme did not leave much time to tourist excursions, however all participants enjoyed the sight of the sea and the friendly atmosphere of the meeting. A quite rich social dinner closed the 3-day event.

All participants (see snapshot below) were very grateful to Maurizio D'Auria and his group (University of Basilicata) for the perfect organization of the scientifically profitable event and enjoyed the nice stay in the wonderful Mediterranean scenery.

Sergio Caffieri, Dipartimento di Chimica Farmaceutica, Università di Padova

Aldo Romani and Ugo Mazzucato, Dipartimento di Chimica, Università di Perugia



CONFERENCE REPORTS

4th Workshop “Energy Flow Dynamics in Biomaterial Systems” October 2-5, 2007, Paris, France.

This workshop has been the second meeting of a prospective series of “PRC Workshops” held at the Paris Research Center (PRC) of the University of Florida. The first PRC workshop, on the topic of “Quantum Dynamics of Complex Molecular Systems”, was held on 18- 20 May 2005, and attracted a considerable number of internationally renowned scientists from the theoretical chemistry and molecular physics communities, whose work focuses on complex molecular processes involving surfaces, clusters, solute-solvent systems, materials and biological systems. This first workshop event has led to the publication of a Proceedings volume in the Springer Chemical Physics series (Quantum Dynamics of Complex Molecular Systems, Eds. D. A. Micha and I. Burghardt, Springer (2006)).

This year’s second PRC Workshop, held on 2-5 October 2007, was organized by I. Burghardt (ENS Paris), E. R. Bittner (University of Houston), V. May (Humboldt-Universität Berlin), and D. A. Micha (University of Florida), with support by the European Science Foundation in the framework of the SimBioMa program. This workshop event has continued the general focus on ultrafast phenomena, photochemistry, and quantum dynamical approaches, but specifically aimed to investigate the role of these phenomena in biological and nanostructured systems. The main thrust of the workshop was thus to contribute to developing a unified theoretical picture of electronic excitation energy transfer in biological systems, molecular electronic materials, and biomimetic systems. To this end, the workshop has drawn together researchers from the following fields: (i) Energy transport and quenching in DNA and light-harvesting systems, (ii) energy and charge transfer in organic materials and interfaces, (iii) quantum and mixed quantum/classical dynamics methods for processes in condensed phases, at surfaces, and in spatially extended systems, (iv) quantum chemistry of non-adiabatically coupled systems, (v) time-resolved ultrafast spectroscopies and multidimensional techniques. The general orientation of the workshop was markedly interdisciplinary. While most of the participants were theoretical chemists, physicists and biologists, an important aim was to explicitly make contact to the experimental side; several leading experimentalists in the field were therefore invited.

One of the distinguishing features of this workshop was that a number of the speakers were invited to give more broad “overview” talks that would touch upon both their work and provide a unified background for the subsequent talks of the session. In particular, overview talks were given by Greg Scholes (University of Toronto) on charge and energy transfer dynamics in nanostructured systems, Steve Bradforth (University of Southern California) on dynamics in DNA and biomolecular systems, Shaul Mukamel (University of California at Irvine) on multidimensional spectroscopy, Peter Rossky (University of Austin) on excited state electronic structure and dynamics, Michael Thoss (Technical University of Munich) on quantum properties and dynamics in many dimensions, Raymond Kapral (University of Toronto) on mixed quantum-classical methods, Laura Herz (Oxford University) on electronic dynamics in material systems, Eitan Geva (University of Michigan) on energy transfer beyond Forster theory, and Gianaurelio Cuniberti (Technical University of Dresden) on molecular electronics. By the diversity of topics and the interdisciplinary nature of the workshop, an active dialogue was created between theorists and experimentalists, as well as between theorists specialized in different domains.

Altogether, the workshop comprised close to 50 participants from 9 countries, a number of whom were postdoctoral fellows and students of senior participants. All participants were invited to contribute to a Proceedings volume to be published in Springer's notable "Lecture Notes in Physics" series and many participants have uploaded the slides from their talk to the workshop's web page, <http://www.chimie.ens.fr/UMR8642/Quantique/Workshop2007/>.

A follow-up workshop event at the Paris Research Center is planned for 2009.

Irene Burghardt

Département de Chimie, Ecole Normale Supérieure, Paris, France

CONFERENCE REPORTS

Supramolecular Photochemistry: From Exciplex to Solar Cells August 9-10, 2007, Tampere, Finland.

The aim of the two day seminar was to collect the research colleagues of Helge Lemmetyinen to celebrate his 60 year anniversary, and to use this opportunity to introduce young scientists to the diverse world of supramolecular photochemistry.



The history of photochemistry in Finland is tightly related to the name of Prof. Helge Lemmetyinen. He published his first photochemical study in 1974 [1], and since then he has published over 200 papers in high ranked international journals. He is the head of the Institute of Materials Chemistry, the Dean of the Faculty of Environmental Technology at Tampere University of Technology and the leader of an internationally well known research team in the field of photochemistry. The international activity of Prof. Lemmetyinen is wide covering the memberships of COST Management Committees, of the Executive Committee of the European Photochemistry Association, and other international research organizations and associations.

In view of Prof. Lemmetyinen wide international and national activity it was no surprise that the seminar attracted some of the top scientists on the field of photochemistry and related sciences, who presented

review talks on their recent research activities. All in all there were 84 participants from altogether 9 countries.

The seminar was opened by the Rector of Tampere University of Technology Prof. Jarl-Thure Eriksson and followed by introductory presentation from the organizing committee.

The first session was devoted to photoinduced electron transfer with two speakers, Prof. Mihail Kuzmin (Moscow State University, Russia) and Prof. Shunichi Fukuzumi (Osaka University, Japan). Prof. Kuzmin presented a new approach to mathematical treatment of the electron transfer reaction accounting for the formation of intermediate transition states such as exciplex. Prof. Fukuzumi gave an overview of new supramolecular electron transfer systems recently developed by his group.

Photodynamics session was opened by Prof. Mark Van der Auweraer (Katholieke Universiteit Leuven, Belgium) who devoted his talk to excited state energy transfer and exciton annihilation in rigid structures of perylene imid substituted pentaphenylene derivatives. The subject of excited state energy transfer was further considered by Prof. Lennart Johansson (University of Umeå, Sweden) who presented the extended Förster theory of the energy migration in biomacromolecular structure. Ultrafast dynamics of the excited state processes of metal complexes was the subject of talk of Prof. Antony Vlcek (University of London, UK) which highlighted effects of excited states in photochemical reaction. Dynamics of the photo-generated charges in polymer-fullerene solar cell materials was reviewed by Dr. Tero Kesti (Lund University, Sweden). The advanced time resolved spectroscopy methods widely used in photochemistry research are finding their applications in solid state physics, as was demonstrated

in the presentation of Prof. Markus Pessa (Tampere University of Technology, Finland) by the example of carrier dynamics investigation in quantum well heterostructures.

Diversity of the objects of supramolecular photochemistry was presented in Photoactive compounds and structures session. The session was opened by an overview talk on modern theories of light-matter interaction given by Prof. Tapio Rantala (Tampere University of Technology, Finland), and followed by reports on development in experimental field. Research advances in the chemistry of chlorophylls were reviewed by Prof. Paavo Hynninen (University of Helsinki, Finland). Prof. Franz-Peter Montforts (Universität Bremen, Germany) reported on recent results in selective synthesis of chlorin pigments for photodynamic therapy and artificial photosynthesis. Aqueous responsive polymers and their studies by fluorescence spectroscopy were presented by Prof. Heikki Tenhu (University of Helsinki, Finland). Recent trends in inorganic photochemistry were presented by Prof. Victor Plyusnin (Institute of Chemical Kinetics and Combustion, Russia) by the example of photochromic systems based on coordination of s-radicals with Ni(II) complexes. In the last presentation of the session Prof. Jaakko Puhakka (Tampere University of Technology, Finland) gave an overview of the environmental biotechnology research in Finland and world wide.

One of the strong sides of the supramolecular photochemistry is its ability to shade light on organization and processes found in complex artificial and natural structures, such as self assembled layers and proteins. This topic was addressed in session Characterization of complex structures. Prof. Dimitra Markovitsi (Francis Perrin Laboratory, France) reported photochemistry on self-organized columnar phase and extended research of DNA helices. Photoinduced vectorial electron transfer in Langmuir-Blodgett and Langmuir-Shaeffer organic films was examined in the presentation of Dr. Aleksander Alekseev (General Physics Institute, Russia). Prof. Jouko Peltonen (Åbo Akademy, Finland) reported on the thermodynamic characterization of lipid and polymer films using various techniques including high resolution probe microscopy. An overview of nonlinear optical techniques for characterization of organic thin films was presented by Prof. Martti Kauranen (Tampere University of Technology, Finland).

The two-day seminar was concluded by the presentation of Prof. Helge Lemmetyinen. He outlined the recent state of supramolecular photochemistry research at Tampere University of Technology, which ranges from ultrafast spectroscopy of complex donor-acceptor systems to solar cell application.

The organizing committee has received many positive responses from the participants of the seminar, both from speakers and young participants. This indicates a growing interest to the field of supramolecular photochemical in Finland and world wide.

The members of the organizing committee would like to express their thanks to all who participated in the seminar.

References

[1] Flash photolysis of acetone in gas phase. Kinetics of ethane formation from methyl radicals. Pohjonen, Marja L.; Leinonen, Leila; Lemmetyinen, Helge; Koskikallio, Jouko., *Finnish Chemical Letters* (1974), **6**, 207-9.

Elina Vuorimaa-Laukkanen
and Nikolai Tkachenko

Institute of Materials Chemistry, Tampere University of Technology, Finland

INVITATIONS

XXII IUPAC Symposium on Photochemistry July 28th to August 1st, 2008, Gothenburg, Sweden

Correspondence

More information, as it becomes available, will be posted on the Symposium website:

<http://photoscience.la.asu.edu/Goteborg2008/>

Correspondence should be sent to:

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First Announcement

XXIInd IUPAC SYMPOSIUM
ON PHOTOCHEMISTRY



GOTHENBURG, SWEDEN
JULY 28 — AUGUST 1, 2008



Invitation

Dear Colleagues

On behalf of the organizing committees, we cordially invite you to attend the XXII IUPAC Symposium on Photochemistry.

The Symposium will be held in the Gothenburg Convention Centre, Gothenburg, Sweden, from 28 July to 1 August, 2008. This will be the latest in a long series of successful symposia, carrying on a tradition of premier biennial gatherings of scientists with interests in photochemistry and related subjects. We look forward to seeing you at this stimulating meeting.

Devens Gust, Chair
Bo Albinsson, Chair of the Local
Organizing Committee

Scientific Program

The symposium will provide a framework for presentation and discussion of ideas and information on the interaction of light and matter drawn from the following areas:

- Organic and inorganic photochemistry from a synthetic and mechanistic point of view
- Solar energy conversion
- Materials science and engineering
- Supramolecular chemistry and nanotechnology
- Photobiology and biophysics
- Photomedicine

- Photonics and imaging
- Spectroscopy and instrumentation
- Photochromism
- Industrial applications of photochemistry and photophysics

The scientific program comprises plenary lectures, invited lectures, contributed oral presentations, and poster sessions. Presenters will be drawn from a wide variety of countries.

Plenary Lecturers

The following distinguished scientists have agreed to present plenary lectures.

Vincenzo Balzani (University of Bologna)
Harry Gray (California Institute of Technology)
Leif Hammarström (Uppsala University)
Stefan Hell, (Max Planck Institut für Biophysikalische Chemie)
Masahiro Irie (Kyushu University)
Josef Michl (University of Colorado)
Atsuhiko Osuka (Kyoto University)
Eric Vauthey (University of Geneva)

Venue

Founded in 1621, Gothenburg, Sweden's second largest city, is a port on the West coast, in the heart of Scandinavia. It is the home of Chalmers University of Technology and Gothenburg University. The climate is mild at the end of July. The

Convention Centre is centrally located close to hotels, restaurants and shops. The city has an extensive and reliable public transportation system. A variety of excursions for accompanying persons are planned.

Visa Information

IUPAC sponsorship implies that entry visas will be granted to all *bona fide* chemists provided application is made not less than three months in advance. If a visa is not granted one month before the meeting, the IUPAC Secretariat should be notified without delay by the applicant.

Registration and Call for Papers

Contributed papers will be accepted as oral or poster presentations. Details and information concerning registration, abstract submission, deadlines, housing and fees will be posted at a later date on the Symposium website:

<http://photoscience.la.asu.edu/Goteborg2008/>

Conference Language

The official language of the Symposium will be English. Simultaneous translation will not be provided.

5th European Meeting on Solar Chemistry and Environmental Applications SPEA 5, October 4th to 8th, 2008, Palermo, Italy



5^o European Meeting on SOLAR CHEMISTRY AND
PHOTOCATALYSIS: ENVIRONMENTAL APPLICATIONS
(Palermo October 4th – 8th 2008)



The “Schiavello – Grillone” Photocatalysis Group is pleased to send you the first circular regarding the 5th edition of SPEA to be held in the city of Palermo (Chairman: Prof. Leonardo Palmisano; co-Chairman: Prof. Vincenzo Augugliaro) from October 4th to October 8th 2008.

The Congress, open to young and well experienced scientists, engineers and the industrial sector will focus on the latest advances and current state-of-the-art in the field of Environmental Applications of Solar Chemistry and Photocatalysis. The following topics will be addressed in the Congress:

1. Water treatment and disinfection
2. Air treatment
3. Soil remediation
4. Green synthesis by solar-chemistry
5. Development of new materials for photochemistry and photocatalysis
6. Developments and perspectives in environmental photochemistry
7. Commercial applications
8. Environmental management
9. Experimental standardization
10. Models for photochemistry and photocatalysis

Finally we hope that it will be a very pleasant time spent with friends and colleagues.

Programme

The conference programme will consist of four plenary lectures and about 40 short communications, complemented by a poster exhibition. Those wishing to contribute are invited to submit abstracts. The Scientific International Committee will select contributions for oral or poster presentation. Although the programme will focus on the main topics listed above, those who wish to present interesting results from other fields of Solar Chemistry and Photocatalysis are encouraged to apply. One page abstracts in MS Word format should be submitted by e-mail to the editorial office: spea5@yahoo.it before May 2nd 2008. Posters or oral communications will be accepted if at least one of the authors is registered at the congress. Authors will be notified about the acceptance and selection for oral/poster presentation by June 2nd 2008. We have scheduled the publication of special issues of two high impact factor International Journals (Catalysis Today and another journal to be selected). All papers submitted will be refereed. Authors interested to the publication in these special issues are invited to submit a full paper before the end of the Conference.

Location

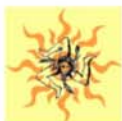
The venue of the meeting is in the Splendid Hotel “La Torre” that is located in Mondello, a part of Palermo still wrapped in the myths of the “belle-epoque” and which is placed between an unexpected traditional fishing village and one of the most beautiful and fascinating beaches of the Mediterranean. However, Mondello is just a few minutes bus ride away from the city centre on the other side of the wide avenues of “Favorita” park. On the opposite side, a short stretch of motorway connects Mondello to the Palermo “Falcone-Borsellino” International airport. The “La Torre” complex is situated after the large semi-circular beach of Mondello, just a few metres on the other side of the fishing village, on a little promontory of which the hotel occupies the smaller part, overlooking the bay with its park stretching out in the opposite direction as far as the “Capo



Splendid Hotel “La Torre”



Swimming pool inside “La Torre”



*5^o European Meeting on SOLAR CHEMISTRY AND
PHOTOCATALYSIS: ENVIRONMENTAL APPLICATIONS*
(Palermo October 4th – 8th 2008)



Gallo" coastal reserve. Over there you will find all aquatic sports (sailing, windsurfing, water-biking, motor-boating, diving, etc).

Further details on the Hotel can be found at www.latorre.com.

Important dates

Friday May 2nd 2008: Deadline for submission of abstracts;

Monday June 2nd 2008: Acceptance of the abstracts and communication to the authors of the modality of presentation (Poster or Oral);

Monday June 16th 2008: Deadline for reduced conference fees payment;

Monday June 30th 2008: Deadline for hotel reservations;

Saturday October 4th 2008: Arrival, accommodation and registration;

Sunday October 5th 2008: Registration, social excursion, welcome cocktail;

Monday October 6th 2008: Plenary lectures, oral communications and poster sessions; meeting of the Scientific International Committee;

Tuesday October 7th 2008: Plenary lectures, oral communications and poster sessions; social dinner;

Wednesday October 8th 2008: Plenary lectures, oral communications, closing session and deadline for submission of full papers.

Conference facilities

The conference hall will be equipped with PC connected to a multimedia projector and overhead projector for powerpoint presentation or slide projection. Authors are recommended to prepare their oral presentation on CD or on USB pendrive. Posters should be exhibited on standard 100x120 cm (LxH) sheets.

Refreshments will be provided in a room behind the Conference Hall. Posters will be displayed in a hall near the Conference Hall, making possible their viewing and discussion throughout the conference. The registration desk will be open for information and assistance throughout the conference.

Accompanying persons:

Visits to the most important landmarks near Palermo (e.g., Segesta, Erice, Agrigento etc) will be scheduled (the excursion will be carried out only if a minimum number of participants is reached). The relative costs will be published on the website prior to the conference.

Transport

Palermo "Falcone-Borsellino" airport is well-served with regular flights from the main Italian cities (Milan, Turin, Rome, Bologna) and from many European cities (e.g. Madrid, London, Paris, Budapest). The connection between the airport and Hotel La Torre Mondello (about 20 km) will be by bus, by metro/bus or by taxi (ca. 50 euros).

Bus transfers to the Hotel "La Torre" from and to the airport will be scheduled on Saturday October 4th 2008 (about at 8.00 PM) and on Wednesday October 8th 2008 (after the closing session). All the information will be available on the conference website <http://spea5.altervista.org/>.

Weather

Weather in Sicily is usually pleasant, sunny and calm during October, but sometimes little rain occurs. Temperature ranges between 15-25°C.



*5^o European Meeting on SOLAR CHEMISTRY AND
PHOTOCATALYSIS: ENVIRONMENTAL APPLICATIONS*
(Palermo October 4th – 8th 2008)



Accommodation

Apart Hotel La Torre other accommodations are available in Mondello or in the downtown. All the information about accommodations, in Hotel La Torre or otherwise, and/or flight tickets, transfer from/to the airport and excursion will be provided by the following agency:

	<p>SERVIZITALIA 90143 Palermo Via S. Puglisi, 15 Tel. +39 0916250453 Fax +39 091303150 info@servizitalia.it reservation.spea5@servizitalia.it www.servizitalia.it</p>
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Visa requirements

A list of countries whose passport holders require visas to enter Italy can be found at:
http://www.esteri.it/visti/home_eng.asp

Medical and travel insurance

It is recommended that all the participants and accompanying persons arrange their own medical and travel insurance for the duration of the conference and field excursion; if requested "SERVIZITALIA" agency can provide the insurance.

Costs (in Euros)

	Before June 16 th , 2008	After June 16 th , 2008
Participants	550 €	650 €
Students (*)	300 €	350 €
Scientific International Committee Members	400 €	400 €
Accompanying persons	200 €	230 €

(*) A declaration of the tutor is requested.

The registration fee will cover the costs of the organization expenses, book proceedings, welcome cocktail, 3 working lunches (October 6th, 7th and 8th), coffee-breaks and taxes (ca. 20%). It will not cover other meals, personal extras and dinners. The fees for the accompanying persons include the social excursion, welcome cocktail, 3 working lunches (October 6th, 7th and 8th), coffee-breaks and taxes (ca. 20%).

Language

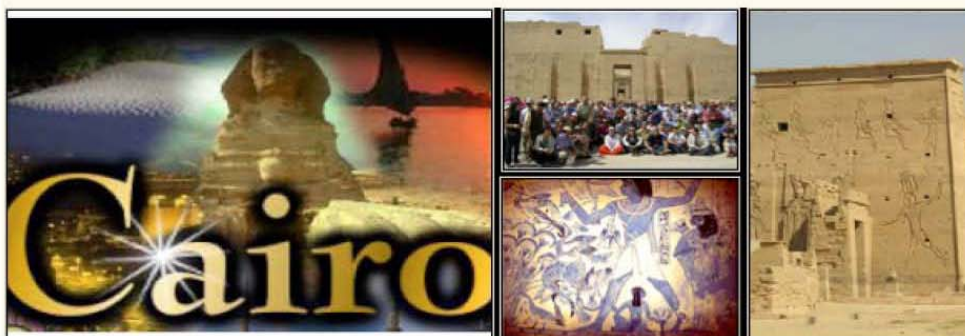
The official language of the congress will be English.

Further Information

Further information will be provided in the 2nd circular and call for papers in December 2007. Information is available also at the following address: <http://spea5.altervista.org>.

Solar Energy Conversion Solar 08, February 24th to 28th, 2008, Cairo, Egypt.

International Conference on Molecular/Nano-Photochemistry, Photocatalysis and Solar Energy Conversion Solar'08 Cairo, Egypt, February 24 –28, 2008



Invitation:

We invite you and the members of your research group to join us in Egypt as we meet to discuss in an interdisciplinary sense the newest trends, break-through, discoveries and applications in photochemistry, photocatalysis, solar energy conversion, environmental aspects and related nanoscience and nanotechnology. The conference will open up channels to gain partners and innovative ideas for new collaborative scientific projects.

Attractive social/cultural and accompanying persons program will be organized.

The scientific program includes Plenary-, Keynote-, Short-Lectures and Poster presentations.

In case you intend to take part actively, please send us a note indicating your personal information; contacts as well as your preferred type of presentation and its tentative title.

Looking very much forward to seeing you in Cairo during the conference.

*Prof. Dr. Sabry AbdelMottaleb
(Chairman, ASU, Egypt)*

Conference Secretariat:

Egyptian International Conferencing; and (Sabry KG, Germany).

Fax: +202 2634 7683 or +202 2638 9725;

Tel: +2010 168 6244

Phochem08@photoenergy.org

Further information at: <http://www.photoenergy.org>

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**HRSMC Summer School on Photochemistry,
May 31st to June 4th, 2008, Maastricht, Netherlands.**



Holland Research School
of Molecular Chemistry



HRSMC Summer School on Photochemistry

The next HRSMC Summer School on Photochemistry will be held in Kasteel Vaeshartelt, Maastricht from May 31 until June 4 2008. For more information on the lecturers and topics please go to http://www.hrsmc.nl/schoolEPA08_programme.html and check out the other web pages with information on this summer school.

Registration is open via http://www.hrsmc.nl/schoolEPA08_registration.html. Please note that your registration must be done **before February 25, 2008**. After that we cannot guarantee a room in the Castle.

Kind regards,

Hilde Zwaan - van der Plas
HRSMC / +31 - (0)20 - 525 6956 / www.hrsmc.nl

Scientific Organizing Committee

prof. dr Fred Brouwer (University of Amsterdam), dr. Francesco Buda (University of Leiden),

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HRSMC Organizers (University of Amsterdam)

Ineke Weijer, drs Hilde Zwaan-van der Plas

Electronic Excited States in Condensed Phases, June 18th to 22nd, 2008, Sicily, Italy.



Workshop announcement and call for contributions

Electronic Excited States in Condensed Phases

ESCOP08

18-22 June 2008

Hotel Santa Tecla

Sicily, Italy

The conference is organized by the COST Action D35 and the ESF DYNA Network with the aim to bring together European scientists interested in electronic excited-states of chemical and biological systems, their structural dynamics, theory, and design of new photoactive systems.

The meeting will cover various aspects of excited-state behavior in a range of photoactive systems, namely molecular and supramolecular systems, metal complexes, conductive polymers, nanoparticles and their interfaces with molecular chromophores, biomolecules (especially peptides and proteins), and complex functional systems (photosynthesis, vision, molecular photonic devices, *etc.*). The scientific topics will include:

- Experimental and theoretical characterization of electronic excited states
- Excited-state structural dynamics
- Relaxation processes and dynamic interactions with the medium
- Electron and energy transfer, bond breaking, isomerization

Bringing together scientists with diverse experience and expertise under the **unifying theme of excited states and their ultrafast dynamics** is expected to stimulate further development of this field in Europe. To facilitate the synergy and cross-fertilization between various research directions, the lecture and poster presentations will be complemented by several discussion sessions.

The conference will be held in a sea-side hotel Santa Tecla (www.hotelsantatecla.it) on the eastern coast of Sicily, north of Catania. The venue was selected with the intention to provide a

nice and pleasant environment, with ample opportunities for informal discussions. Top tourist cultural and natural sites, such as Taormina or Mt. Etna, are nearby.

No conference fee will be charged to any participant. The size of the meeting is limited to 70-80 participants. COST D35 and ESF DYNA will provide a number of bursaries to cover travel and subsistence costs. The bursaries will be allocated by the organizing committee based on the scientific quality and relevance of submitted contributions. Applicants will be asked to submit abstracts by 31 December 2007.

The organizers invite all prospective participants to submit the preliminary registration form before the end of June 2007. The form can be downloaded from:

<http://www.jh-inst.cas.cz/escop08/>

All inquiries concerning this meeting should be sent by e-mail to the contact address: chemistry-d35@qmul.ac.uk

We are looking forward to seeing you in Sicily,

Organizing committee:

Prof. Antonín Vlček
Queen Mary, University of London
Chair of the COST Action D35 "*From Molecules to Molecular Devices*"

Prof. Majed Chergui
Ecole Polytechnique Fédérale de Lausanne
Chair, ESF Research Networking Programme "*Ultrafast Structural Dynamics in Physics, Chemistry, Biology and Material Science*" (DYNA)

Prof. Sebastiano Campagna
Università di Messina

Ing. Lucie Víchová
J. Heyrovský Institute of Physical Chemistry, Prague

8th International Conference on Pulse Investigations in Chemistry, Biology and Physics PULS'2008, September 6th to 12th, 2008, Kraków, Poland.



www.ichtj.waw.pl/puls2008

8th International Conference on Pulse Investigations in Chemistry, Biology and Physics PULS'2008

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e-mail: puls2008@ichtj.waw.pl

Łódź / Warszawa, December 5, 2007

Charge transport in various media

Heterogeneous systems

Ionic liquids

Ionization tracks and high mobility systems

Polymeric systems

Radicals and radical ions in biological systems

Transients in gases

Ultrafast reactions and relaxation dynamics

Water and aqueous solutions at ambient and high temperatures

Dear Colleagues:

We are pleased to send you the 1st Announcement for the 8th International Conference on Pulse Investigations in Chemistry, Biology and Physics PULS'2008 to be held in Kraków, Poland from September 6 through September 12, 2008.

For additional information about the Conference, please see our web site at:

<http://www.ichtj.waw.pl/puls2008>. This web site will be updated as new information becomes available. Please forward this announcement to anybody you might think is interested in attending the conference.

We look forward to your participation in the 8th PULS conference, and please contact us via e-mail: puls2008@ichtj.waw.pl if you need further information.

Best regards,

Krzysztof Bobrowski

Jerzy L. Gębicki

Conference Co-chairmen



The Faculty of Chemistry
Institute of Applied Radiation Chemistry
TECHNICAL UNIVERSITY OF ŁÓDŹ

Department of Radiation Chemistry and Technology
Pulse Radiolysis Group
INSTITUTE OF NUCLEAR CHEMISTRY AND TECHNOLOGY



UPCOMING MEETINGS

2008

□ **Central European Conference on Photochemistry**

February 10-14, 2008

Bad Hofgastein, Austria

Website : <http://www.ptc.tugraz.at/gastein/>

□ **Solar Energy Conversion Solar 08**

February 24-28, 2008

Cairo, Egypt

Website : <http://www.photoenergy.org>

□ **16th Ultrafast Phenomena Conference**

June 9-13, 2008

Stresa (Maggiore Lake), Italy

Website : <http://www.ultraphenomena.org>

□ **Electronic Excited States in Condensed Phases ESCOP08**

June 18-22, 2008

Sicily, Italy

Website : <http://www.jh-inst.caz.cz/escop08>

□ **XXII IUPAC Symposium on Photochemistry**

July 28-August 01, 2008

Göteborg, Sweden

Website : <http://photoscience.la.asu.edu/Goteborg2008/>

□ **5th European Meeting on Solar Chemistry and Environmental Application, SPEA 5**

October 04-08, 2008

Palermo, Italy

Website : <http://spea5.altervista.org/>

MEMBERSHIP APPLICATION FORM



EUROPEAN PHOTOCHEMISTRY ASSOCIATION 2008 MEMBERSHIP RENEWAL/APPLICATION FORM

Please complete the form and send it to the Treasurer (by fax, mail or e-mail):

Dr. Silvio Canonica EAWAG, W+T Dept.
Ueberlandstrasse 133, P.O. Box 611, CH-8600 Dübendorf, Switzerland
(Fax +41 44 823 5210, E-mail: canonica@eawag.ch)

I wish to renew/apply for membership of the European Photochemistry Association (EPA)

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