Supramolecular Chemistry and Photochemistry of Materials

I. Research Group

The group of **Supramolecular Chemistry and Photochemistry of Materials** of the Faculty of Chemical Technology and Engineering, UTP University of Science and Technology in Bydgoszcz is inviting researchers to cooperate. The group is comprised of three different divisions: (1) Division of Organic Chemistry, (2) Division of General and Inorganic Chemistry constituting Department of Chemistry and (3) Division of Chemical Technology and Physical Chemistry of Materials.

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Faculty of Chemical Technology and Engineering
Seminaryjna 3, PL-85-326 Bydgoszcz, Poland

II. Group's Leader

Group leader: Borys Ośmiałowski
About: born 1973, working in research since 1997,

- M.Sc. in the topic of photophysical properties of Schiff bases (synthesis, photophysical properties, hydrogen bonding and charge transfer research),
- Ph.D. in the topic of tautomerism of heterocyclic compounds (synthesis, measurements, DFT computations),
- post-doc at the University of Zurich in group of prof. Kim Baldridge and prof. Jay S. Siegel
- D.Sc. in the topic of supramolecular chemistry (synthesis, DFT computations, multinuclear NMR spectrometry)
- currently interests (experiments and calculations): *a*) tautomerism, *b*) hydrogen bonding, *c*) fluorescent compounds, *d*) molecular probes, *e*) conformational equilibria in supramolecular chemistry.

Webpage:http://kcho.utp.edu.pl/BO/Welcome.html
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III. Group's Members and Research Interests

- Borys Ośmiałowski (supramolecular chemistry, BF_2-carrying molecules, fluorescent probes, DFT computations, hydrogen and halogen bonding, substituent effects)

- Małgorzata Kaczorowska (application of HRMS and MS/MS (ECD, EDD, ETD, CID) methods for structural elucidation of supramolecular species, metal ions complexes, peptides, proteins and their post-translational modifications, polymers),
- Janina Kabatc (polymethine dyes, photosensitizers, photoinitiators, photopolymerization - thermodynamic and kinetic studies),
- Beata Jędrzejewska (photophysical properties of molecules in their excited states, photoinitiated polymerization and isomerization, sensibilization in radical photoinitiated polymerization, styryl dye synthesis)
- Agnieszka Skotnicka (tautomerism in CH-acids, substituent effect, organic synthesis)
- Robert Dobosz (DFT computations, proton transfer reactions)
- Marek Pietrzak (chalcones and azachalcones synthesis, spectroscopic and polymerization kinetics measurements)
- Karina Mroczyńska (supramolecular chemistry, hydrogen bonding, DFT computations, IR spectroscopy)
- Izabela Grela (multinuclear NMR spectrometry, solid state NMR)

IV. Leading Research Topic of the Group

In general, our group is interested in structure-property relationships in the light of various properties of organic molecules. These are: a) electron transfer, b) substituent effects, c) benzannulation, d) proton transfer reactions (mainly tautomerism), e) photophysical and photochemical properties of molecules, f) intermolecular interactions, g) photopolymerization.

V. Description of Main Research Topic

To be more specific the following list describe briefly main research trends:

Electron transfer

In our group we are interested in the intramolecular charge transfer and its influence on photophysical properties of organic compounds but also intermolecular one that is applied in initiation of radical polymerization. These mechanisms are studied experimentally and with the use of quantum-chemical calculations.

Substituent effect

The substituent effect is present in many fields of science. We have focused on electronic and steric effects on intermolecular interactions but also on the influence of substituent on photophysical properties in fluorescent molecules that may also isomerize upon interaction with light.

Benzannulation

The benzannulation (together with the wider concept of “aromaticity”) is a well known way to change the molecular properties by introduction of the benzo ring fused with other ones. Since benzannulation (Clar rule) play a role in electron distribution it is used in tuning the absorption/fluorescence of molecules and ability of those to initiate polymerization.

Proton transfer reactions

Proton transfer is a process that may take place, both, in ground state and excited state of molecules. In our group we are mainly interested in ground state proton transfer. This may be divided into intramolecular one (tautomerism) and intermolecular (yielding salts).

Photophysical and photochemical properties

The research in this topic is based on the processes that acts between molecules and within them. The charge transfer that can be tuned by modification of molecular topology is studied in the light of tuning the absorption and emission of heterocyclic compounds in regular way. This research is devoted to better understand the basic properties that can be used in, for example, photoinitiated reactions.

Intermolecular interactions

The supramolecular approach to properties of organic molecules we use is mainly focused on the properties of hydrogen bonded complexes and their flexibility. Even the rotation around single bonds are important in the field. Thus, the isomerization and its influence on intermolecular interactions is researched with the use of electronic and steric effects within supramolecular complexes.

Photopolymerization

In this field, we are focused on photoinitiated polymerization and any aspects related with this process. The main purposes of the research are to develop new one- and more components initiating systems effective in visible and infrared light and to understand processes that result from the light absorption.

The mentioned research areas are explored by us with the use of experimental and DFT-based calculations methods.

VI. General Expression of Interests

Our general interests are focused on physicochemical properties of organic compounds. These include: synthesis of a) organic dyes and b) compounds capable for intermolecular interactions. Regarding point ‘a’ we are interested in heterocyclic compounds that may be used in, for example, photoinitiated polymerization or as a molecular probes. Point ‘b’ refers to the self-organization of organic compounds in solution but also in solid state.

VII. Specific Interests and Additional Topics of Extended Interest

We are looking for cooperation in the following fields: molecular probes, fluorescent indicators, supramolecular complexes, photoinitiated polymerization and supramolecular chemistry and photochemistry in general. We are also open to new topic of research that is loosely related to our main interests.

VIII. Other Important Characteristics of the Group

All members of the group are highly motivated in the field of research and open for external cooperation. We welcome persons interested in similar topics to contact us via e-mail or by phone (or personally of course). The techniques we usually use in everyday work is: multinuclear NMR, electronic absorption, fluorescence, transient absorption, time resolved fluorescence, photo-calorimetry, cyclic voltammetry

Apparatus (except equipment used in organic synthesis): NMR (lowered temperatures, solid state, nuclei: ^{1}H, ^{11}B, ^{13}C, ^{15}N, ^{19}F), differential scanning calorimetry, photo-DCS, spectrophotometers UV-Vis, spectrofluorimeters (lowered temperatures, solid state), time-correlated single photon counting (TCSPC) system spectrometer , nanosecond laser flash photolysis, cyclic voltameters.

For a recent information about ongoing projects see:

- https://www.researchgate.net/project/Fluorescent-difluoroborates
- https://www.researchgate.net/project/Intermolecular-interactions-in-the-light-of-DFT-computations
- https://www.researchgate.net/project/Conformational-equilibrium-in-supramolecular-chemistry
- https://www.researchgate.net/project/New-photoinitiators-acting-under-visible-light-for-radical-polymerization

IX. Main Group's Achievements

Synthesis of compounds interacting with the use of hydrogen bonds and synthesis and measurements of compounds used in photoinitiated polymerization. We have published ca. 220 scientific publications in peer-reviewed journals. For full list have a look at Web of Science.

X. Chosen publications

Below we mention few very recent publications:
RSC Adv. (2016) **6**, 103851, Dyes Pigm. (2016) **130**, 226, Dyes Pigm. (2017) **136**, 150, J. Org. Chem. (2015) 80, 9641, J. Phys. Chem. A, (2016) **120**, 4116, J. Org. Chem. (2013) **78**, 7582, J. Org. Chem. (2016) **81**, 2280, Beilstein J. Org. Chem. (2015) **11**, 2105, Int. J. Mass. Spectrom. (2015) 389, 54, J. Am. Soc. Mass. Spectr. (2013) **24**, 1224.