Summaries of the main results and scientific contributions of Dr. Nikolay Iliev Georgiev, presented for the competition for the position of professor

Assoc. Prof. Georgiev's publication activity includes 78 articles, 71 of which are in international journals with an impact factor (total impact factor 282.6). In the current competition, he is participating with 29 publications with a total impact factor of 107.9. According to SCOPUS data, Assoc. Prof. Georgiev's scientific output has been cited 1517 times in foreign journals and series (h-index = 26 according to SCOPUS, excluding self-citations). Notably, these scientific metrics have been achieved with an average annual teaching load of over 400 hours. Additionally, Dr. Georgiev is actively involved in advising graduate students. Since his habilitation, he has supervised 47 theses. He has authored over 100 reviews (75 after his habilitation) for prestigious international journals with an impact factor, such as Dyes and Pigments, Analytica Chimica Acta, Sensors and Actuators, Journal of Luminescence, Journal of Fluorescence, Spectrochimica Acta Part A, Journal of Photochemistry and Photobiology, ChemistrySelect, and Journal of Materials Chemistry.

Dr. Nikolay Georgiev's research focuses on the design and synthesis of functional fluorescent compounds from the classes of 1,8-naphthalimide, 9-phenylxanthene, and perylene. He has synthesized a large number of new, previously undescribed compounds. He investigates their photophysical behavior and their potential applications as molecular sensors and molecular logic devices for rapid diagnostics in analytical chemistry, biology, and medicine.

The scientific and applied contributions of Dr. Georgiev's presented works can be grouped into several main research areas:

1. Synthesis and investigation of new multichromophore systems for energy transfer at the molecular level

Light plays a vital role in human life, serving as the primary energy source for living organisms and the most accessible energy source in nanotechnologies for constructing molecular machines and devices. Therefore, designing and synthesizing molecular systems capable of effectively capturing and transporting light energy represent a significant scientific interest. In natural photosynthetic systems, a vast array of chlorophyll molecules surrounds a reaction center. The remarkable feature of these photosynthetic systems is that the energy of each photon absorbed by these antenna complexes is transported with over 90% efficiency through Förster Resonance Energy Transfer (FRET). FRET is a process in which an excited donor fluorophore transfers energy to an acceptor dye in the ground state without emitting a photon. This process is distance-dependent and typically requires effective spectral overlap between donor emission and acceptor absorption.

In his work, Dr. Georgiev focuses on the synthesis of PAMAM (polyamidoamine) [26] and benzyl ether [21,23] light-harvesting architectures containing 1,8-naphthalimide donor units. For the first time, benzyl ether light-harvesting systems entirely composed of 1,8-naphthalimide fluorophores have been synthesized and investigated [21,23]. The obtained architectures are a natural extension of his dissertation work, where similar structures based on PAMAM scaffolds were examined. Unlike PAMAM, the benzyl ether architectures avoid the presence of photoinduced electron transfer (PET), which would render their fluorescence signaling pH-sensitive. For this reason, to obtain a pH sensor antenna in the central acceptor fluorophore, a PET receptor fragment has been introduced, and the resulting antenna has been successfully applied as a sensor for proton determination. Additionally, for the first time, the occurrence of twisted intramolecular charge transfer (TICT) has been observed in the 1,8-naphthalimide units upon their incorporation into benzyl ethers via the C-4 position of the fluorophore. Due to the strong sensitivity of this phenomenon to the presence of water molecules, the obtained results have been applied to develop fluorescent sensor systems for detecting the presence of water in organic solvents.

Furthermore, the idea of synthesizing benzyl ether light-harvesting antennas is further expanded, resulting in a light-harvesting antenna capable of transporting light energy to a 1,8-naphthalimide rotor with a switching mechanism [21]. This marks the first deliberate combination of a light-harvesting system, molecular rotor, and molecular switch into a multi-component molecular device.

2. Synthesis and investigation of novel fluorescent molecular sensors

Developing new materials with programmable properties at the molecular level is a strategic priority of the EU to promote research in the fields of chemistry and materials science over the next decade. Designing organic molecules capable of serving as molecular sensor devices is expected to significantly improve human life conditions by enhancing healthcare, providing the opportunity for rapid and precise detection of extremely low concentrations of highly toxic or pathogenic entities, both in living organisms and in the environment.

Molecular systems in which fluorescence is "switched" between "on" and "off" states under the influence of external chemical stimuli can be designed according to several principles. In Dr. Georgiev's work, fluorescent sensor molecules operating via photoinduced electron transfer [1,7,9,10,15,16,20,23,27,28], intramolecular charge transfer [1,4,8,9,13,20,22,24,25,26], fluorescence resonance energy transfer [1,13,17,19,27], intramolecular proton transfer [2,3,5,14,17], and the formation of excimers [18,29] have been synthesized and investigated. All resulting products serve as excellent indicators for detecting protons, and some of them also have the potential for determining Cu^{2+} [1-3,6,7,10,14,22,25,27], Hg^{2+} [7,8,10,19,22,25,27], Fe^{3+} [19,22,25], Al^{3+} [22], Pb^{2+} [1], Ni^{2+} [22], S^{2-} [6,22], CN^{-} [22], and F^{-} [22]. Fluorescent sensor molecules for detecting water content in organic solvents [18,23] and determining viscosity [4,21] have also been obtained.

2.1. Synthesis and investigation of novel water-soluble sensor molecules

The major drawback of fluorescent sensors is that they primarily function in organic environments and do not provide any analytical response in aqueous environments. Consequently, the number of commercial fluorescent sensors on the market is still relatively small, and there has been a recent strong demand in the field for synthetic methods to obtain water-soluble molecules. In Dr. Georgiev's work, new highly water-soluble PET sensor systems based on 1,8-naphthalimide and perylenediimide have been synthesized and investigated [4,7,9,10,15]. It has been established that they can selectively determine the pH of the medium in 100% aqueous solutions. This categorizes the new sensor molecules as environmentally tolerant indicators. Interestingly, the new perylenediimide, besides exhibiting high water solubility, also demonstrated good cellular penetration and low cytotoxicity, making it highly suitable for diagnostics in medicine and biology [7].

Synthetic approaches to creating water-soluble organic products are often associated with heavy, lengthy, and tedious multistep reactions. A relatively new approach to overcoming this problem is the incorporation of hydrophobic organic products into polymeric water-soluble micelles. This approach has also been utilized in Dr. Georgiev's work to impart water-soluble properties to perylenediimide and 1,8-naphthalimide molecules [28,29]. As a result, water-based fluorescent micelles have been obtained, exhibiting excellent pH sensor properties. It has been found that the new fluorescent micelles possess good cellular penetration and low cytotoxicity, making them a promising diagnostic indicator in medicine and biology.

2.2. Synthesis and investigation of novel solid-state emitting PET sensing 1,8-naphthalimides

The photoinduced electron transfer based on the "fluorophore-spacer-receptor" format is the most popular approach used in designing fluorescent chemosensors. In recent years, a wide variety of chemosensors based on photoinduced electron transfer have been synthesized, and the phenomenon has been extensively studied for the detection of various analytes in solutions. At the same time, reports on solid-phase PET sensor materials are extremely rare. For the first time, in the works of Dr. Georgiev, PET sensor 1,8-naphthalimides emitting in the solid-state have been synthesized and investigated. During the examination of thin films, it was found that the PET process occurs in unsubstituted, 4-halogenated, and 4-alkyloxy-substituted PET 1,8-naphthalimide systems. Thanks to this, films of these compounds have been successfully applied as chemosensors for the rapid detection of acidic and basic vapors. Additionally, they exhibit excellent reversibility, which suggests their repeated use in practice.

3. Synthesis and investigation of novel molecular logic devices and apparatuses

The minimization of semiconductor elements has already reached its limit, hence the design of molecular devices capable of performing logical operations has gained broad interest. In semiconductor devices, logical elements operate through a binary system, encoding signals as 0 and 1 (low and high voltage). This process is feasible at the molecular level in several ways, but currently, it is most commonly achieved through the optical properties of fluorescent molecular sensors, by using low and high concentrations of guest molecules as input and detecting the fluorescent intensity of the output product (weak emission-0 or strong emission-1). Molecular logic devices are of interest for applications such as smart materials in object encoding, drug delivery, and rapid diagnostics.

Dr. Nikolay Georgiev is the first Bulgarian scientist to focus his scientific interest on the application potential of molecular sensors as molecular logic devices. In his works, the following basic logical functions at the molecular level have been implemented: OR [4,19,27], INH [6,13,14,20,22,27], XOR [6, 20], AND [6,19,22], IMPLICATION [13,14,20], XNOR [20], NAND [22], NOR [22], and three-input INH [25].

In his work, Dr. Georgiev managed to obtain molecular-level comparison devices (digital comparators) through all possible logical paths [3,9,12,14,17,20]. He reports on achieving the digital comparator by using two INH [9] molecular gates and the possibility of obtaining a digital comparator through negative molecular logic (replacing INH with IMPLICATION). He authored the first tutorial review on molecular digital comparators, where he explains, in accessible language, not only the principles applied in building comparison devices but also the fundamental mechanisms used in the field of molecular logic [12].

Dr. Georgiev is one of the few scientists who expand and popularize the idea of AP DeSilva, where sequentially linked AND or INH at the molecular level are respectively considered as an enabler and disabler. He constructs at the molecular level Input3, Input4-doubly disabled INH [10], and a magnitude digital comparator with a disable option [2]. Additionally, he synthesizes and reports for the first time the logical gate Disabled-Enabled-OR at the molecular level, operating through 4 inputs.

Scientific publications of Dr. Nikolay Georgiev

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5. Sakr A.R., Georgiev N.I., Bojinov V.B. *Synthetic Communications*, (2020) **50** 2988 - 2996.

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