

In XIX and XX centuries spectacular progress not only in organic chemistry but also in inorganic chemistry and metallurgy was achieved. These two last domains significantly contributed to the emergence of electronics and its subsequent progress. Electrical, electrooptical and magnetic properties of organic compound had not drawn significant attention of the scientific community for many years. This attitude changed in 1973, after the discovery of peculiar electrical properties of TTF-TCNQ - the first organic metal. Consecutive discoveries in the domain of organic metals and semiconductors led Alan J. Heeger, Alan G. MacDiarmid and H. Shirakawa to the Nobel prize in chemistry in 2000. Organic semiconductors offer several properties unobtainable for their inorganic counterparts: i) they are lighter; ii) they show strong anisotropy of physical properties; iii) their electrical, electrooptical and magnetic properties can be tuned by appropriate functionalization; iv) attaching appropriate solubilizing groups renders them solution processable. For these reasons organic semiconductors have been applied as components of active layers in various electronic devices such as field effect transistors (FETs), light emitting diodes (LEDs) photovoltaic cells (PC), photodiodes (PD) and others.

The main goal of this proposal is the design, synthesis and determination of physical properties of new solution processable organic semiconductors as well as the fabrication of test FETs and LEDs considered as a proof of concept. An important scientific novelty element in this research is the use of over 100 years old and almost forgotten intractable alizarine-type dyes in the preparation of solution processable organic semiconductors from the azaacene family. From the materials chemistry, physical chemistry and electrochemistry stand point nonlinear azaacenes are extremely interesting compounds. Depending of the N/C ratio in the conjugated core electrical transport properties of azaacenes can be tuned from n-type to ambipolar (n- and p-type). This also involves their spectroscopic properties, including emissive ones. Preliminary studies showed that solution processable nonlinear azaacenes, can be relatively easily obtained from indanthrone, a vat dye, in a simple one-pot process consisting of the reduction of the carbonyl group followed by the substitution with solubility inducing alkoxy groups under phase transfer catalysis conditions. These new compounds show excellent self-organizing properties and high electroluminescence.

Their dibromoderivatives will be used as building blocks in the synthesis of new donor-acceptor semiconductor of DAD or ADADA structures, including molecules active in thermally activated delayed fluorescence, TADF. The TADF process has recently been extensively studied since its application leads to LEDs of significantly improved efficiency.

In the synthesis of these compounds various C-C coupling reactions will be exploited (Suzuki, Stille, Sonogashira and others). All new azaacenes as well as DAD and ADADA compounds will be investigated by electrochemical and spectroelectrochemical (UV-vis-NIR, EPR, Raman) means with the goal to elucidate their redox properties and to determine their ionization potential (IP) and electron affinity (EA) values - the parameters playing an important predictive role in applications of organic semiconductors. 3D supramolecular organization will be determined in single crystal and thin layers by X-ray diffraction. Self-assembly properties and the 2D structure of monolayers will be investigated by scanning tunneling microscopy (STM). The fabrication of test FETs and LEDs will be treated as a proof of concept.

Spintronics is a new kind of electronics exploring spin of unpaired electron. Up to now no stable organic materials exhibiting spins polarization have been obtained. In the frame of our project we plan the design, the synthesis and the magnetic properties studies of new organic high-spin materials. These materials should contain two types of alternating units, i.e. units bearing unpaired electron spins and units coupling spins in ferromagnetic fashion. The spins ordering causes the increase of intrinsic magnetic moment and the appearance of magnetic interactions. We will use aromatic oligoamines oxidized to radical cations as spin bearing units. Spin coupling units will be composed of meta-benzene and its derivatives. These studies allow determining the main rules for designing high-spin organic compounds. Special attention will be paid to spins interaction spread along linear polymer chain.