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Highly efficient **NIR** organic emitters with **inve**rted **s**inglet-**t**riplet excited states (***NIR-INVEST***)

My vision is the implementation of a rationally designed **NIR-INVEST** - organic materials which will fundamentally alter the trends in the design of efficient, low in energy light sources, anchoring a new paradigm in NIR semiconductor technology.

Motivation: Energetically low near-infrared (**NIR**) light exhibits superior optical penetration, lesser photodamage, and lower optical scattering compared to high in energy, visible light. For this simple reason, NIR-emitting organic materials have found a potential interest in bioimaging, night-vision technologies and advanced optoelectronics. However, the low efficiency of their emission caused by the energy gap law hinders considerably the exploration of modern optoelectronic materials to be put as the cornerstone of the "*Internet-of-things*" (IoT). Inspired by this challenge, the goal of this project is to develop the synthesis semiconductors with inverted singlet-triplet excited-state energies (**INVEST**), which is a violation of the text-book Hund's rule, as a new class of low-energy optoelectronic materials with unprecedented performance. Their structure promotes spontaneous radiative relaxation of the entire population of available excitons under NIR-shifted emission (> 900 nm) while neglecting the energy gap law, hereby constituting a novel concept termed: **NIR-INVEST**.

The aim of research: To tackle this challenge, I will combine the design and the synthesis of conceptually new 2D organic materials with unprecedented efficiency of energetically non-invasive NIR emission owing to the unusual configuration of singlet-triplet excited states. I aim at maintaining the stability of inversion within strong chromophores with distinct structures, to reveal a mechanistic rationale behind an INVEST phenomenon which is the key to achieve a large bathochromic shift of the emission, keeping its efficacy intact regardless of a solution and solid-state environment. Merging ST inversion with a high throughput of NIR-emitted light will allow me to come up with a new paradigm for low-energy consuming, organic photosemiconductive technology. To achieve my research objectives and experimentally prove the hypothesis, the synthesis and analysis of aza-polycyclic architectures in which **INVEST** will be persistent. NIR emission will be tuned by core modification involving its integration with distinct but well-defined assemblies embracing (a) functional dyes, (b) interlocked macrocycles, and (c) 2D nanotubes and 3D Mackay-type aza-carbon allotropes. Such a unique combination of **INVEST** and NIR emission will provide an access to (a) a fundamental understanding of **INVEST** mechanisms and use of dyes as novel class of OLED emitters, (b) development of NIR lightning in aqueous conditions, and (c) aggregation-free solid-state individual emission, with largely shifted NIR emission caused by the synergic effect.

Expected impact of the research project: The scientific output of this project will have an impact on the research society involved in emissive organic π-conjugated architectures considering a revolutionary conceptualization of the efficient and deep NIR shifted emission by violation of the excited-states features. Since organic materials with on-demand engineered emissions have become appealing for optoelectronic devices, ground-breaking research envisaged in this project will attract an interest of physicists and biologists seeking for a low-energy-consuming, durable, and intense source of light produced for security vision, NIR-light emitting diodes, and IoT.