The resurgence of interest in polycyclic aromatic hydrocarbons (PAHs) arises from both the desire to investigate the relationship between their structure-function properties and their increasing application in modern technology such as photonics and molecular electronics. Engineering of novel fluorescent probes/materials and the application graphene, fullerenes, and nanotube derivatives play a crucial role. The current drawbacks of PAHs are limited to their regioselective functionalization as well as their photo- and thermostability.

One potential solution may be to construct PAH analogs based on a nitrogen heteroaromatic scaffolds with reduced electron density. Currently, nitrogen-doped rigid aromatic systems garner considerable research interest, given the possibility of creating various interactions with other molecules. These materials easily protonate in acidic conditions and solvate with various metal ions. Both processes modify the electronic structure of the material, and consequently, its fluorescent properties. However, progress in this field is constrained by synthetic difficulties in creating materials with a precise defined structure.

A key aspect of the grant application is developing a method for their synthesis based on the latest synthetic techniques by employing mechanosynthesis. This method focuses on the transformation of covalent bonds in chemical molecules induced by the mechanical force generated during the grinding of reactants in an appropriate ball-mill reactor. Mechanochemistry represents a fourth way of inducing chemical reactions, complementing thermal reactions in fluids, photochemistry, and electrochemistry. It is gaining attention due to its short chemical reaction times, solvent free, energy savings, and high yields of the products formed. In addition to these practical benefits, mechanochemical synthesis using ball milling has the potential to provide exciting opportunities to access large areas of previously unexplored chemical space where the reactivity of chemical species may differ from that occurring in conventional solutions.

The synthetic strategy will be based on the production of N-doped compounds with a polyphenyl structure of various sizes and shapes, which will then be planarized via a ball mill in a process called cyclodehydrogenation. In the final stage, all obtained materials will be thoroughly examined, determining the impact of N-doping of aromatic hydrocarbons on their photophysical properties.

The tangible goal of the project will be to discover new, unprecedented aromatic architectures with unique photophysical properties. Increased stability of the newly formed structures, compared to their carbon analogs, is expected due to their increasing electron-deficient nature. The inclusion of pyridine units, or other azines in a polyaromatic system with a $\pi$-extended structure, will provide a unique family of tunable internal fluorophores, where changes in electronic polarization, solvation, and coordination will translate into dramatic alterations in their photophysical properties. This will lead to significant contributions to the development of useful chemosensors and new light-emitting materials. Particular emphasis will be placed on constructing appropriate complexes with transition metals to obtain better NIR OLED emitters. Emission in this range is invisible to humans, but the produced materials may be useful in applications related to fiber optic communication.