

Despite many unique features, single walled (SWCNT) and multiwalled carbon nanotubes (MWCNT) suffer from low hydrophilicity, difficult processability, incompatibility with most polymer matrices and low fluorescence quantum yields, *etc.*, which restricts their application portfolio and makes them unfit for some practical fields. Thus, carbon nanotubes (CNT) are often surface-modified – functionalized – by suitable functional groups to enable attachment of various organic and inorganic substances in order to enrich their properties and, hence, the application potential of the resulting hybrid system. The covalent decoration with molecules may tune physicochemical features of the carbon nanomaterials due to synergetic effects and bring new properties that are not present in the pristine carbon nanostructures. For example functionalized SWCNT are used as an important element of transparent, bendable screens for smartphones, while conductive inks based on MWCNT allow printing of conducting paths on textiles enabling development of “smart” clothing. Thus, new functionalization protocols and reactions for enhancement and modification of CNT properties are still needed to be developed as they might allow realization of even more advanced projects.

One of such reactions which potentially allow control over optical and electronic properties of CNT is [2+1] cycloaddition of organic nitrenes as it shows unique diameter-dependent regioselectivity. For example, CNT of diameter larger than 2.4 nm are predicted to form selectively “closed-configuration” adducts which have disturbed local conductivity and enhanced fluorescence properties while adducts with CNT of small diameter, so called, “open-configuration” will preserve local conductivity. Use of organic nitrenes, especially phenyl nitrenes due to presence of phenyl ring, possibly allows modification of electronic properties of “open-configuration” adduct through preserved and extended conjugation on phenyl ring substituents. Both adducts might have extraordinary influence on the optical properties of semiconducting single walled carbon nanotubes (scSWCNT) which show unique emission of fluorescence in near infrared region. That property can be utilized in biomedical imaging or single quantum transfer of information but it still has to be enhanced. The another advantage of [2+1] cycloaddition of nitrenes is undiscovered potential of introducing complex organic molecules on scSWCNT surface which might be used in development of new therapeutic and diagnostic tools in medicine. Results of the project will expand scope of modifications of SWCNT for a new reaction which enables engineering electron and optical properties of carbon nanotubes.

The project is a relevant part of current research on the modification of electron, optical and physical properties of carbon nanotubes through structurally well-defined chemical functionalization. The research results of the project might potentially lead to development of new materials for NIR OLED diodes used in military technologies or novel fluorescent probes for biomedical imaging in II-NIR window.