

Nanochemistry and Nanobiotechnology

Binding of *meso*-Tetrakis(*N*-methylpyridinium-4-yl)porphyrin to poly(rI)·poly(rC)–SWNT hybrid

G.O. Gladchenko¹, M.V. Karachevtsev¹, V.V. Andrushchenko², V.S. Leontiev¹, V.A. Karachevtsev¹

¹ *B. Verkin Institute for Low Temperature Physics and Engineering, Natl. Acad. of Sci. of Ukraine, 47 Lenin Ave., 61103 Kharkov, Ukraine*
E-mail: gladchenko@ilt.kharkov.ua

² *Institute of Organic Chemistry and Biochemistry, Acad. of Sci., Flemingovo nam.2, 16610 Prague, Czech Republic*

For improving the solar cells, new materials are required that will provide better current transfer. Material that has emerged as a strong contender is single walled carbon nanotube (SWNT). Due to the decoration of SWNT with porphyrins which have unique chromophoric features, novel building blocks for photovoltaic nanodevices can be developed. However, to prepare functional SWNT-based nanocomposites, it is necessary to solve the problem involving main steps: 1) to create DNA–SWNT hybrid and to ensure the hybrid stability in an aqueous suspension; 2) to ascertain major mechanisms of porphyrins coupling with the hybrid.

In the present work the binding of *meso*-Tetrakis(*N*-methylpyridinium-4-yl)porphyrin (TMPyP4) to nanohybrids formed by SWNT with double-stranded poly(rI)·poly(rC) (rI·rC) has been studied using absorption spectroscopy and molecular dynamics simulation. Hybrids were obtained by means of a) (rI·rC) adsorption to SWNT and b) hybridization of poly(rI) and poly(rC) on the nanotube surface. It is shown that duplexes hybridized on SWNT are characterized with the structure defectiveness and, as a result, the reduced stability in comparison with that hybridized without the nanotube or (rI·rC) adsorbed to the nanotube surface. The latter was chosen as the main sample for research.

Results demonstrate that TMPyP4 interacts with (rI·rC)–SWNT nanohybrid. After the addition of TMPyP4 into (rI·rC)–SWNTs suspension the Soret band demonstrated the red-shift with respect to the free dye. The spectral shift depends on TMPyP4 concentration: the maximal shift (~20 nm) is observed at low porphyrin concentrations (10^{-6} – 10^{-5} M) and is gradually decreased to 14 nm at $3 \cdot 10^{-5}$ M TMPyP4. Such behavior of the Soret band is interpreted in terms of different types of porphyrin binding with (rI·rC)–SWNT, including π – π -stacking interaction of the porphyrin core with the nanotube surface as well as the electrostatic interaction between the cationic group of the *N*-methylpyridyl ring and the negatively charged phosphate group of (rI·rC).