**Investigation of the dynamics and structure of nanomaterials used in medicine**

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***Abstract:***

The present work is devoted to the investigation of the structure and dynamics of nanomaterials by neutron scattering, UV-vis spectroscopy, and dynamic light scattering methods.

Fullerenes were chosen as the nanomaterials under study. It is already known, that fullerenes exhibit a variety of non-typical physical-chemical properties, such as solvatochromic effect, unusual thermal and concentration dependence of optical parameters, solubility with anomalous thermal dependence, etc. The cause for all these phenomena is claimed to be the aggregation of fullerenes, yet the mechanisms of fullerene cluster formation and transformation are still not properly described. Special properties of fullerenes are the most relevant and valuable for medicine. Usage of fullerenes in medical treatment naturally requires the creation of aqueous fullerene solutions. Understanding the processes of transition of fullerenes into liquid medium and discovering means to control formation of clusters is an important step towards improving the methods of obtaining the aqueous solutions with sized-down aggregates of fullerenes. Apart from that, the research of fullerenes C70 alongside fullerenes C60 opens up the possibility to create absolutely new methods of obtaining aqueous fullerene solutions and their further application in medicine. Considering that aqueous fullerene solutions are made by transferring the fullerenes from non-polar solvent into water, the aim of the project is to explore the behavior of fullerenes and their clusters in liquid systems with consequent change of polarity.

To reach this purpose the following methods are going to be used: neutron scattering, dynamic light scattering and UV-vis spectroscopy.

***Tasks:***

1. Understanding of the scientific problem.

2. Studying methodologies.

3. Plotting the distributions of cluster sizes by intensity, mass, and volume.

4. Plotting the dependences of optical absorption on wavelengths.

5. Processing of raw-data small-angle neutron scattering spectra.

***Preliminary schedule by topics/tasks:***

The duration of this project is 5 weeks.

***1-3 weeks***: Introductory talks:

* characteristics of nanomaterials
* possibilities of studying the structure and dynamics of matter
* small-angle neutron scattering methods,
* X-ray diffraction,
* inelastic neutron scattering,
* UV-view spectroscopy,
* dynamic light scattering

***3-4 weeks***: Data processing

***5th week***: Preparation and writing a report

***Required skills:***

1. Basic knowledge of condensed matter physics.

2. Basic knowledge of neutron / X-ray scattering methods.

3. Basic knowledge of spectroscopy methods.

4. Computer skills: OriginPro.

***Acquired skills and experience:***

1. Understanding the problems of clusterization of nanoparticles used in medicine

2. Influence of polarity on the size of aggregates in liquids.

3. Skills at small-angle neutron scattering.

4. Ability to interpret data obtained by UV-vis and DLS methods.

***Recommended literature:***

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2. I. Natkaniec, D. Chudoba, Ł. Hetmańczyk et al. Parameters of the NERA spectrometer for cold and thermal moderators of the IBR-2 pulsed reactor, Journal of Physics: Conference Series, 2014, vol. 554, 012002;

3. Nagorna T., Kuzmenko M., Kyzyma O., Chudoba D., Nagornyi A., Tropin T., Garamus V.M., Jazdzewska M., Bulavin L.: Structural reorganization of fullerene C70 in N-methyl-2-pyrrolidone / toluene mixtures. Journal of Molecular Liquids. 272, 948-952 (2018).

4. Nagorna T.V., Kyzyma O.A., Chudoba D., Nagornyi A.V.: Temporal solvatochromic effect in ternary C70/toluene/N-methyl-pyrrolidine-2-one solution. Journal of Molecular Liquids. 235, 111-114 (2017).

5. Якимова Л.С. Метод УФ-спектроскопии и его применение в органической и физической химии. Казань: Казан. ун-т, 19 с (2015).