

IR absorption spectroscopy of carbon dots to elucidate the relationship between their photoluminescence and structure

Vervald A.M.¹, Laptinsky K.A.^{1,2}, Khmeleva M.Yu.¹, Dolenko T.A.¹

¹Faculty of Physics, M.V. Lomonosov Moscow State University, Moscow, Russia

²Skobeltsyn institute of nuclear physics, M.V. Lomonosov Moscow State University, Moscow, Russia

IR absorption spectroscopy is one of the most common methods for the study of the structure of carbon dots (CDs). This method provides rich information about interatomic vibrations in nanosystems and allows drawing conclusions about the presence/absence of certain intermolecular bonds in their structure. Unfortunately, the relationship between such vibrations and the most interesting property of these nanoparticles, their photoluminescence, has not yet been investigated.

In this study, to elucidate the relationship between the photoluminescence of carbon dots and their structure investigated via IR absorption spectra, a large array of 343 different carbon dots was studied. CDs were synthesized from citric acid and ethylenediamine using the hydrothermal method with smoothly varying synthesis parameters – synthesis temperature and time, precursor ratio. For all nanoparticles, IR absorption spectra and photoluminescence spectra were obtained. The calculated values of the photoluminescence' quantum yield of the obtained particles varied from fractions to more than 95%. Along with a change in the intensity of CDs photoluminescence, a change in the intensity and position of bands in their IR absorption spectra was also found. The observed bands were identified and interpreted, the changes in the characteristics of the IR absorption bands and their dependence on the synthesis conditions and the concentration of precursors were analyzed, and the correlation of certain IR absorption bands with the intensity of CDs photoluminescence was shown. As a result of the work, conclusions were drawn about the correspondence between the photoluminescent characteristics of CDs and the structural features of nanoparticles due to different synthesis conditions.

This study has been conducted at the expense of the grant of the Russian Science Foundation № 23-72-01042, <https://rscf.ru/en/project/23-72-01042/>