A LUMINOPHORES BASED ON COMPLEXES OF BIOPOLYMERS AND SILVER CLUSTERS: REVEALING OF THE STRUCTURE USING QM/MM MODELS AND THE DATA OF LUMINESCENCE SPECTROSCOPY.

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Silver clusters no larger than 2 nm in size, stabilized by a biopolymer matrix, are widely regarded today as promising luminophores for the creation of biomarkers in vivo [1]. Exciting in UV range a small silver clusters, whose dimensions are limited by the stabilizing matrix, exhibit high luminescence luminosity and photostability in a wide range of visible spectrum with a large quantum yield. Despite a significant increase in the number of experiments in this field for the last decade to date there are no general ideas about the structure of the luminophore obtained and about the prerequisites for their growth.

In our work, we applied an approach [2] based on a comparative analysis of the experimental and calculated excitation and luminescence polarization spectra of the structures under study. Theoretical structures were obtained during the calculation of equilibrium configurations of complexes of silver clusters with full-size biopolymer matrices (DNA and proteins) in a real water-salt environment using the combined QM / MM scheme. As a result of the work, it is shown that, depending on the structure of the matrix, the shape of the luminescing cluster can be either extended linear or spherical, and the structure of the luminescing cluster can contain from 3 to 10 silver atoms in different degrees of oxidation. The reported study was funded by RFBR according to the research project No.16-32-00293.

References

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