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DOXORUBICIN SORPTION/DESORPTION ON MODIFIED SILICA-MAGNETITE NANOCOMPOSITES

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Abstract. A series of new nanocomposite (NCs) based on Fe_3O_4 magnetic nanoparticles coated with SiO_2 (NCs **1**,**2**) (or aminated SiO_2, NCs **3**,**4**) as a new materials for drug delivery (for example, doxorubicin (Dox)) were synthesized (Figure 1).

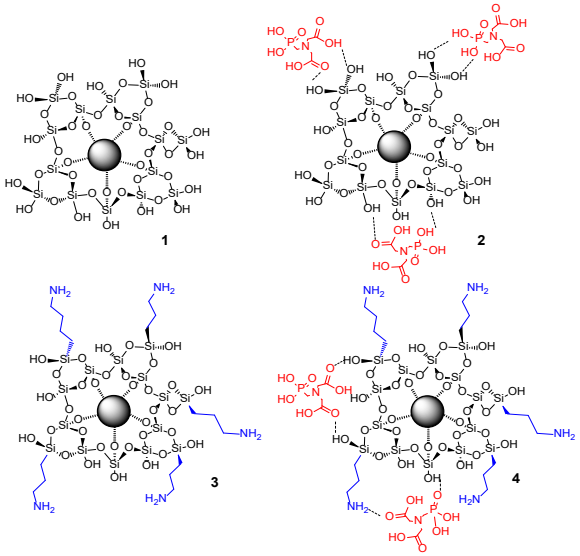

Figure 1. Schematic imaging of synthesised NCs **1**-**4**.

It has been demonstrated for the first time that the presence of PMIDA on the surface of NCs increases the level of Dox loading due to specific binding, while surface modification with 3-aminopropylsilane, on the contrary, significantly reduces the sorption capacity of materials. These regularities were in accordance with the results of quantum chemical calculations. Based on the DFT simulation, the mechanisms of Dox binding to the surface of NCs were proposed: simultaneous coordination of Dox on the PMIDA molecule and silanol groups at the NC surface leads to a synergistic effect in Dox binding. The synthesized NCs exhibited pH-dependent Dox release, as well as dose-dependent cytotoxicity in in vitro experiments. NCs with a SiO_2 shell obtained using PMIDA exhibited the highest effect.[1, 2] We believe that the data obtained can be further used to develop stimuli-responsive materials for targeted cancer chemotherapy.

References

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2. Demin A. Design of SiO_2/aminopropylsilane-modified magnetic Fe_3O_4 nanoparticles for doxorubicin immobilization / A. Demin, A. Vakhrushev, M. Valova [et al.] // *Russian Chemical Bulletin. – 2021. – Vol. 70, Iss. 5. – P. 987-994.*

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