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Study of the local atomic structure of silver ions in silicate glasses based on X-ray absorption spectroscopy and computer modeling by using density functional theory.

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Noble metal nanoparticles are of great interest for a wide range of disciplines due to their unique optical properties. In particular, silver nanoparticles exhibit strong light absorption in the UV range. This phenomenon arises due to the plasmon resonance effect, which can be configured by changing the synthesis technology.
To predict the properties of the final product one has to understand the mechanisms which are responsible for forming this product.
Despite the fact that the growth process of silver nanoparticles is being actively investigated, we have to pay additional attention to the fixing process of silver ions in glass and the formation of initial stable structures. One of the possible mechanisms for the fixing of silver ions can be so-called hole traps centers. Their study is hampered by the amorphous glass structure. In this work we propose an approach to determining the local atomic structure of silver ions in glass matrices with the help of computer modeling by using density functional theory methods which are supported by X-ray absorption spectroscopy.
To get the initial parameters we will use the EXAFS analysis and then we will verify our results by comparing the calculated XANES spectra with the experimental data.

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Author: Mr DURYMANOV, Veniamin (Aleksandrovich)

Co-authors: Mrs SUKHARINA, Galina (southern federal university); Prof. BUGAEV, Lusegen (southern federal university); Mrs BAZOVAYA, Sofiya (southern federal university); Mr KAPTELININ, Sviatoslav (Yurievich); Mr SRABIONYAN, Vasiliy (southern federal university)

Presenter: Mr DURYMANOV, Veniamin (Aleksandrovich)

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