

A Multimodal Approach to Quantify Surface Functional Groups and Ligands on Amorphous Silica Nanoparticles

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Nowadays amorphous silica nanoparticles (SiO₂-NP) are one of the most abundant engineered nanomaterials, that are highly stable and can be easily produced on a large scale at low cost. Surface-functionalized SiO₂-NP are of great interest in the life and material sciences, as they can be used e.g. as drug carriers, fluorescent sensors, and multimodal labels in bioanalytical assays and imaging applications. Their performance in such applications depends not only on particle size, size distribution, and morphology, but also on surface chemistry, i.e. the total number of surface functional groups (FG) and the number of FG accessible for subsequent functionalization with ligands or biomolecules, which in turn determines surface charge, colloidal stability, biocompatibility, and toxicity.[1] Aiming at the development of simple, versatile, and multimodal tools for the quantification of many bioanalytically relevant FG and ligands, we investigated and compared various analytical methods commonly used for FG quantification (Figure 1). [2,3] This includes electrochemical titration methods, dye-based optical assays, and other instrumental analytical techniques such as nuclear magnetic resonance and thermal analysis methods.

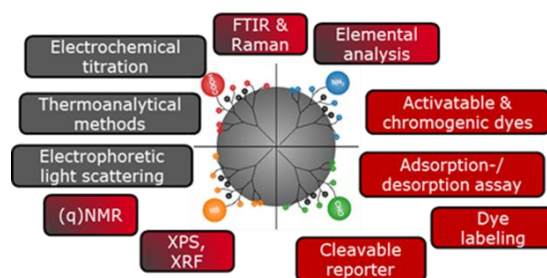


Figure 1. Analytical methods commonly used to quantify the total number of FG (grey) and accessible number of FG (red) present on the NP surface.

The potential of our multimodal approach for FG quantification was demonstrated for commercial and custom-made silica particles of varying FG, showing not only an influence of the synthesis methods on the number of FG but also on the performance. In the future, our strategy can contribute to establish multi-method characterization strategies to provide a more detailed picture of the structure-properties relationship.

[1] I. Tavernaro, S. Dekkers, L. G. Soeteman-Hernández, P. Herbeck-Engel, C. Noorlander, A. Kraegeloh, *NanoImpact* 2021, 24, 100354.

[2] D. Geißler, N. Nirmalanathan-Budau, L. Scholtz, I. Tavernaro, and U. Resch-Genger, *Microchimica Acta* 2021,188, 321.

[3] N. Nirmalanathan-Budau, B. Rühle, D. Geißler, M. Moser, C. Kläber, A. Schäfer, U. Resch-Genger, *Sci. Rep.* 2019, 9, 17577.