IMPACT OF THE CRYSTAL STRUCTURE OF SILICA NANOPARTICLES ON RHODAMINE 6G ADSORPTION

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Silicon is one of the most abundant elements on Earth with around 78% of Earth's crust consisting of various silicon and oxygen compounds [1]. Due to this, silica nanoparticles (SNPs) are widely used nanostructures for drug delivery, bonding and coating applications and others [2].

The properties of nanoparticles strongly correlate with their size hence it is critical to have an accurate way of measuring it. Commonly used techniques such as small angle x-ray scattering (SAXS), transmission electron microscopy (TEM) or dynamic light scattering (DLS) have drawbacks, such as being expensive and requiring complex sample preparation. Additionally, they might be inaccurate for particles under 10 nm size.

Potential methods that can be used to measure sizes of such constructs are time-resolved fluorescence anisotropy [3], and fluorescence recovery after photobleaching (FRAP) however, due to the size of the system it is impossible to determine experimentally how the dye is oriented on the SNP surface. As a result, its contribution to the measured complex size is unknown. Fortunately, the dye and SNP interaction mechanism can be studied using computational methods, such as molecular dynamics, which allow full insight into such processes on an atomistic scale.

In this work we used molecular dynamics simulations to get an insight into the rhodamine 6G (R6G) adsorption process to assess the most favourable conditions for successful adsorption and determine the impact of the dye to the measured complex size. Furthermore, we found that due to the geometric constraints and the requirement of correct dipole moment orientation, only one R6G molecule can adsorb on any sized SNP, and the R6G layer formation on the nanoparticle surface is not possible. Similar restrictions lead to the fact that the highest stable R6G oligomer is a dimer [4].

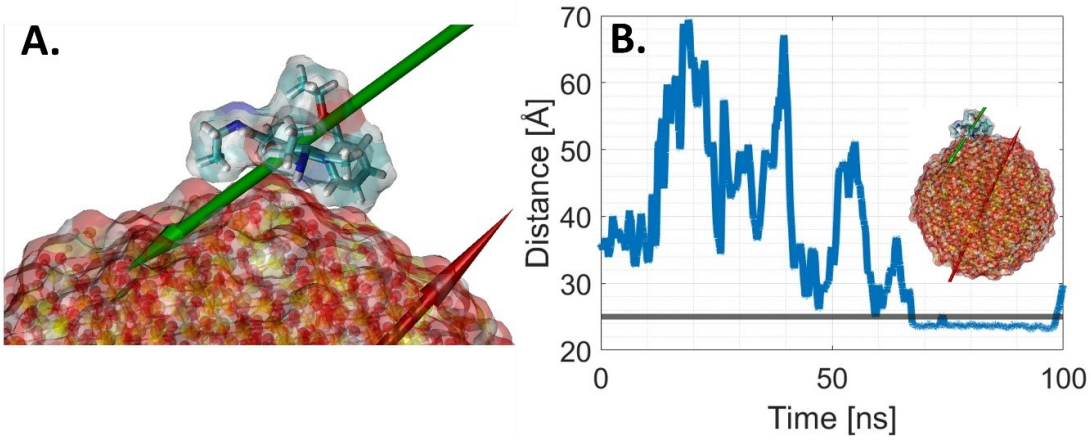

Fig. 1. Rhodamine 6G adsorption on the SNP surface **A.** R6G adsorbed on the surface of the SNP with visualized dipole moments; **B.** Distance plot between centre of masses (COM) of R6G and SNP.

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