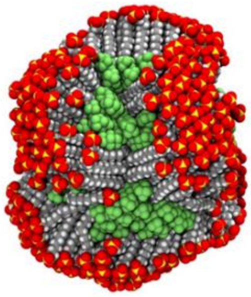
Design, investigation and applications of functionalized ultrasmall silica nanoparticles

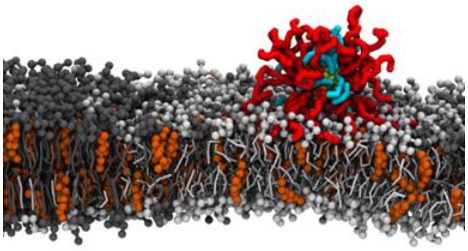
Supervisor: Prof. Lucia Pasquato, e-mail: lpasquato@units.it
Co-supervisor: Prof. Paola Posocco, e-mail: paola.posocco@dia.units.it

Fluorinated nanomaterials have emerged as a fascinating area of research in recent decades. Thanks to the unique properties imparted by fluorine, an element rarely present in biological systems, these materials hold exceptional promise for both therapeutic and diagnostic applications.

Among them, ultrasmall silica nanoparticles (SiNPs) functionalized with fluorinated self-assembled monolayers stand out. As reported for fluorinated (nano)materials, we foresee this surface engineering dramatically enhances their hydrophobicity and stiffness, promotes ordered self-assembly, and drives phase segregation between fluorinated and non-fluorinated components. Such features open the door to a wide range of applications, from bioimaging contrast agents and drug delivery systems to advanced sensors and even solutions for PFAS remediation.



This research project is dedicated to advancing the development and understanding of such functionalized SiNPs, with the ultimate goal of unlocking their full potential across these diverse applications. The work brings together two complementary approaches: experimental investigations and molecular modeling studies. This synergy will provide deep insights into the structure–property relationships of these nanosystems, paving the way toward the design of next-generation fluorinated nanomaterials tailored for specific uses.



The hosting groups offer extensive expertise in the synthesis, characterization, and testing of nanomaterials [1] (Prof. L. Pasquato) as well as molecular modeling of nanosystems [2] (Prof. P. Posocco), supported by a long-standing and productive collaboration.

In addition to these main research directions, and depending on the candidate interests, there will be opportunities to explore exciting additional systems based on gold nanoparticles. Notably, recent work has shown that when these nanostructures, if combined with molecular catalysts, give rise to a groundbreaking class of catalytic systems named as suprazymes [3]. To maximize the capabilities of these innovative materials, the development of tailored computational models will be essential, offering critical insights and guiding the design of future catalytic systems.

The ideal candidate will have a background in theoretical chemistry and synthetic organic chemistry, a strong motivation to push scientific boundaries, and a curiosity-driven approach to learning and discovery. Solid written and spoken English skills are also valuable. The research project can be adapted and tailored based on the candidate developing skills, interests, and the results achieved throughout the course of the research.

References

[1] C. Gentilini, et al., *J. Am. Chem. Soc.* **2008**, *130*, 5678; C. Gentilini, et al., *Angew. Chem. Int. Ed.* **2009**, *47*, 3060; M. Boccalon, et al. *Chem. Commun.* **2013**, *49*, 8794; M. Boccalon, et al. *J. Mater. Chem. B.* **2015**, *3*, 432; D. Marson, et al., *Small*, **2019**, *15*, 1900323; M. Şologan, et al., Nanomaterials, **2019**, 9, 879; E. Pellizzoni, et al. *J. Coll. Interf. Sci.* **2022**, 607, 1373–1381.

[2] C. Gabellini, et al., *ACS Nano*, **2022**, 16, 20902−20914; I. K. Mati, et al., *ACS Nano* **2021**, 15, 8295; Kravets M. et al., *ACS Catal.* **2023**, 13, 24, 15967.

[3] P. Hyziuk, et al., Chem. Sci., **2024**, 15, 16484.