# Friday Materials Science Colloquia #13

Friday, July 19, 12 p.m.
Seminar room, U5 Building – via Roberto Cozzi 55, Milano

Lecturer: **Paulo Siani**

Title: **Mechanistic Insights from Molecular Dynamics Simulations in Nanomedicine**

Abstract: Molecular dynamics (MD) simulation techniques have been at the forefront of recent nanomedicine research, becoming an indispensable tool for unveiling complex molecular mechanisms sometimes beyond the reach of experimental methods. In this talk, I will present how MD simulations can complement existing experimental knowledge and provide new mechanistic insights into relevant aspects of nanoscale devices designed for nanomedicine. By showcasing past and ongoing research projects – from investigating how thermodynamic variables (e.g., pH and ionic strength) affect protein corona formation on organic-functionalized nanoparticles [1], to examining the impact of different degrees of active ligand conjugation on PEGylated nanoparticles for designing more effective targeting nanosystems [2], and utilizing non-equilibrium MD simulations to predict the zeta potential of nanoparticles in solution [3] – this presentation aims to illustrate the utility of classical MD simulations in bridging the gap between simulated microscopic systems and their experimental macroscopic counterparts, thereby encouraging future collaborations.

References:
[1] Siani, Paulo, and Cristiana Di Valentin. *Nanoscale* 14.13 (2022): 5121-5137.
[2] Siani, Paulo, et al. *Journal of Colloid and Interface Science* 627 (2022): 126-141.
[3] Siani, Paulo, et al. *The Journal of Physical Chemistry C* 127.19 (2023): 9236-9247.

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Lecturer: **Irene Tagliaro**

Title: **Engineered chitosan-based materials**

Abstract (max 500 words): Carbohydrates are known for their outstanding structural properties and for being involved in biological surface interactions. Because of the increased sensibility toward a sustainable and circular economy, polysaccharides are becoming increasingly important as row materials for the substitution of fossil-fuel derived products. PFAS, for example, are excellent synthetic chemicals with superior properties of water-repellency which nowadays raised serious concerns for their pervasive use in everyday items that led to significant environmental pollution and toxicity alerts. As in the case of PFAS, there is a urgent demand for developing innovative materials which combines non-toxicity and biodegradability to the desired functional properties of contemporary materials. In this context, polysaccharides emerge as a valuable source of biopolymers. They can be functionally modified to meet specific industrial needs while, at the same time, combining the exploitation of sustainable raw materials well suited for economic circularity. Moreover, biologic carbohydrate-based materials, i.e. exopolysaccharides, offer a platform of bioinspiration for the development of functional properties at interfaces. Among others, chitosan stands out for its non-toxic nature, the potential for functional modification, and its ability to form films. Chitosan-based materials are explored in their properties, especially related to wettability. By chemical modification and engineered processing, chitosan coatings are prepared

as hydrophilic and hydrophobic substrates and tailored for specific applications i.e. anti-icing materials [1], water-repellent coatings [2,3]. For these purposes, the analysis of surface interactions of chitosan with water and ice becomes extremely interesting for understanding of how chemical and structural features of surfaces behaves at interfaces by means of contact angle analysis and ice adhesion strength measurements. This research contributes to the advancement of biopolymer science but also aligns with the global initiative to foster environmentally responsible innovation.

References:
[1] Accepted manuscript at Colloids & Surfaces A
[2] I. Tagliaro et al., Carbohydrate Polymers 302 (2023) 120424
[3] I. Tagliaro et al., Carbohydrate Polymers 333 (2024) 121981