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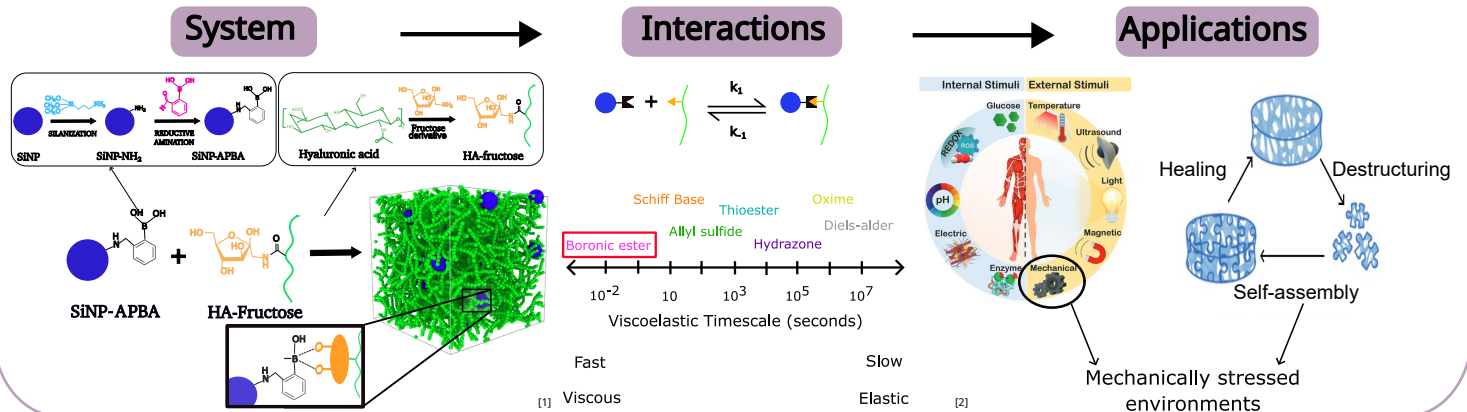
Designing tough and self-healing composite hydrogels for biomedical applications

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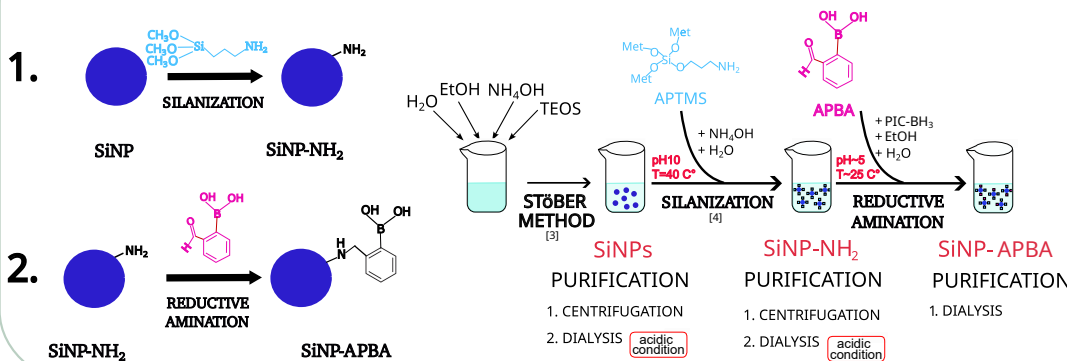
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The exceptional mechanical performance of living tissues is due to their complex and multi-composite molecular structures organized hierarchically in space. Alterations of these microstructures show a significant correlation with age and with many diseases, such as rheumatism or cancerous lesions. In this context, recent advances in biomaterials research have encouraged the design of new biomimetic materials with the ability to resist damage and to regenerate their biological functions under load. Among these materials, nanocomposite hydrogels are promising materials for applications in medicine and tissue engineering. However, controlling their self-assembly to form a self-healing system with high toughness and fatigue resistance remains a major challenge. To overcome this barrier that hinders a technological breakthrough, we aim at developing a novel composite hydrogel composed of hyaluronic acid biopolymers reinforced with inorganic silica nanoparticles (SiNPs) and interacting through dynamic covalent bonds. These strong covalent bonds have rapid assembly and disassembly kinetics, that would help the hydrogel adapt to external conditions while exhibiting high toughness. I will develop a method to functionalize and stabilize SiNPs with appropriate groups to form boronic ester bonds under physiological conditions. In addition, I will show a coarse grained molecular dynamics simulations of a model gel that will be used to investigate the microscopic mechanisms controlling the rheological response.

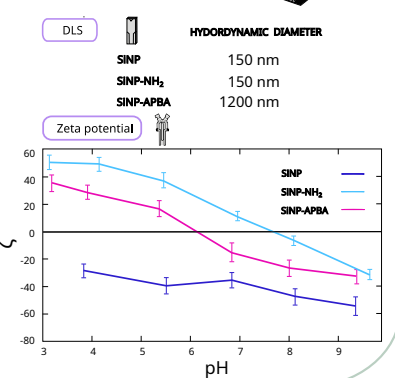
Tough and self-healing hydrogel



SYNTHESIS/FUNCTIONALIZATION



CHARACTERIZATION



Computational model

Coarse-grained model

- Langevin dynamics:

$$m \frac{d^2 \mathbf{r}_i}{dt^2} = \mathbf{F}_i^c + \mathbf{F}_i^f + \xi(t)$$

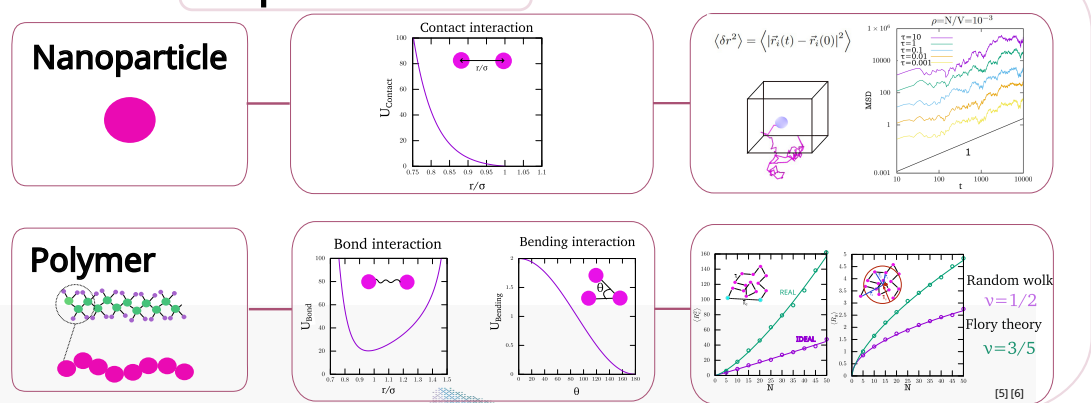
- Truncated and shifted

Lennard-Jones:

- Unit of length: $\sigma = 1$

- Unit of energy: $\epsilon = 1$

- Unit of time units in: $t^* = \sqrt{\frac{m\sigma^2}{\epsilon}}$



Conclusion and outlook

- Synthesis and characterization of SiNP-APBA.
- Study of nanoparticle dynamics and single polymer chain structure through coarse-grained Molecular Dynamic simulations.
- Formation of nanocomposite gel and analysis of the linear and non-linear mechanical response.
- Use of the Molecular Dynamic simulations to probe the microscopic dynamics of the nanocomposite gel.

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