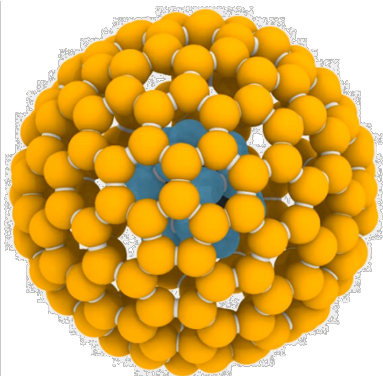


Inside-out activation of Metaparticles



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Background: Transport nanoparticles are engineered particles, typically ranging from 1 to 100 nanometers in size, designed to carry therapeutic agents directly to specific cells or tissues within the body. Metaparticles are nanoparticles responsive to the environment, e.g. they change shape and properties. The "inside-out" activation mechanism refers to the process by which these metaparticles are activated from within, often in response to specific physiological conditions or external stimuli, to release their cargo at the precise location and time needed.

Rationale: Understanding the structural and dynamic mechanisms of inside-out activation will enable the design of controllable, tunable and efficient drug delivery platforms.

Goal:

- Understand the inside-out activation of Metaparticles by means of Brownian dynamics simulations
- Understand the interaction mechanisms between active Metaparticles and the cellular membrane

Research questions

1. How sensitive is a metaparticle to internal stimuli?
2. What are the mechanisms of inside-out activation?
3. What are the interaction mechanisms between active metaparticles and the cellular membrane?

Research approaches

1. Coarse grained simulations (Brownian/Langevin dynamics)
2. Model development with LAMMPS
3. Machine learning

References

1. M.Paesani and **I.M.Ilie***, Metaparticles: Computationally engineered nanomaterials with tunable and responsive properties, *J. Chem. Phys.* **161**, 244905 (2024)

