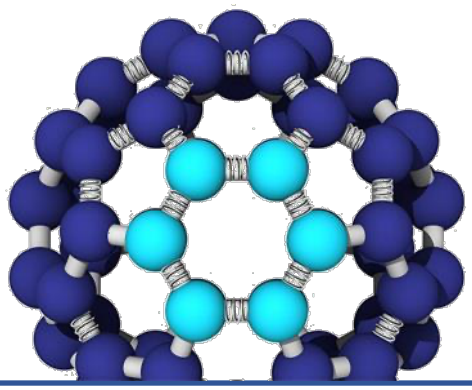
Intelligent Materials: Learning Metaparticles (iMP)



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Background: Intelligent materials (or smart materials) are engineered to respond dynamically to environmental stimuli such as temperature, pressure, light or electric fields. These materials can adapt, self-heal, or change their properties in real-time, making them valuable in advanced applications across medicine, aerospace, robotics, and wearable technology. Intelligent materials are driving innovation in sustainable design, autonomous systems, and next-generation electronics. Metaparticles are nanoparticles responsive to the environment, e.g. they change shape and properties.

Rationale: The computational design of the next generation of Metaparticles, *i.e.* dynamically learning to adjust intrinsic flexibility, size, interactions, depending on the environmental conditions, will enable the development of intelligent materials with brain-like properties.

Goal:

- Computationally develop intelligent Metaparticles (iMPs)
- Understand the physical mechanisms of learning new properties
- Understand how individual iMP properties affect the collective behavior.

Research questions

1. What are the key ingredients to develop an intelligent material?
2. What are the mechanisms of learning?
3. What are the interaction mechanisms between multiple iMPs?

Research approaches

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

References

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

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MULTISCALE SIMULATIONS OF
BIOMOLECULAR SYSTEMS