

Myfanwy Evans (University of Potsdam): Geometry-based simulation of self assembly

Monday, 19 February 2024 14:30 (30 minutes)

The morphometric approach to solvation free energy is a geometry-based theory that incorporates a weighted combination of geometric measures over the solvent accessible surface for solute configurations in a solvent. In this talk, I will demonstrate that employing this geometric technique in simulating the self assembly of sphere clusters and small loops results in an assortment of interesting geometric configurations. This gives insight into the role of shape in the physical process of self assembly, potentially relevant to proteins, viruses and other complex systems.