Simulations of Protein Aggregation

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Abstract:
A number of diseases, known as amyloid diseases, are associated with pathological protein folding. In the case of Alzheimer's disease, incorrectly folded Amyloid-beta (Aβ) proteins self-assemble into a variety of neurotoxic aggregate species, ranging from small soluble oligomers to amyloid fibrils. An attractive therapeutic approach to combat amyloid diseases lies in the development of strategies to inhibit or reverse aggregation. In the first part of my talk, I will present fully atomistic molecular dynamics simulations of the interaction of aggregation inhibiting peptides with Aβ amyloid fibrils. In the second part, I will introduce a novel off-lattice coarse-grained model for the Ab protein and discuss the kinetics and thermodynamics of aggregation and fibrillogenesis inhibition.

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5.521 Levin Hall