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Modeling aggregation of proteins on computers

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Protein aggregation refers to the process by which fully or partially unfolded proteins self-associate to make large and insoluble aggregates. Amyloid fibrils - a prominent example of the aggregates, is implicated in various neurodegenertive diseases and also has found multiple uses in technology. In this talk we will focus on what can be learned about amyloid formation using theoretical models and methods. First, we will give a broad overview of the problems and challenges facing theoretical approaches in the studies of protein aggregation, ranging from the description of small oligomers [1], which are often considered kinetic intermediates to fibrils, continuing on to particlar details of amyloid structure [2]. Then, we will present a model - RAPID - specifically designed for simulations of protein aggregates [3] in water. Finally, we will discuss microscopic details of the aggregation pathway presented by the shortest amyloidogenic peptide reported so far - KFFE [1].

1. A. Baumketner and J. E. Shea, Biophysical Journal 89 (3), 1493-1503 (2005).
2. L. Negureanu and A. Baumketner, Journal of Molecular Biology 389 (5), 921-937 (2009).
3. B. Ni and A. Baumketner, Journal of Chemical Physics 138 (6), 064102 (2012).

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