

Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Molecular insights into early stage aggregation of di-Fmoc-L-lysine in binary mixture of organic solvent and water MD MASRUL HUDA, NEERAJ RAI, Mississippi State University — Molecular gels are relatively new class of soft materials, which are formed by the supramolecular aggregation of low molecular weight gelators (LMWGs) in organic solvents and/or water. Hierarchical self-assembly of small gelator molecules lead to three-dimensional complex fibrillar networks, which restricts the flow of solvents and results in viscous solid like materials or gels. These gels have drawn significant attentions for their potential applications for drug delivery, tissue engineering, materials for sensors etc. As of now, self-assembly of gelator molecules into one-dimensional fibers is not well understood, although that is very important to design new gelators for desired applications. Here, we present molecular dynamics study that provides molecular level insight into early stage aggregation of selected gelator, di-Fmoc-L-lysine in binary mixture of organic solvent and water. We will present the role of different functional groups of gelator molecule such as aromatic ring, amide, and carboxylic group on aggregation. We will also present the effect of concentrations of gelator and solvent on self-assembly of gelators. This study has captured helical fiber growth and branching of fiber, which is in good agreement with experimental observations.

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Date submitted: 13 Nov 2016

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