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A molecular dynamics simulation of *N*-(fluorenyl-9-methoxycarbonyl)-dipeptides supramolecular hydrogel

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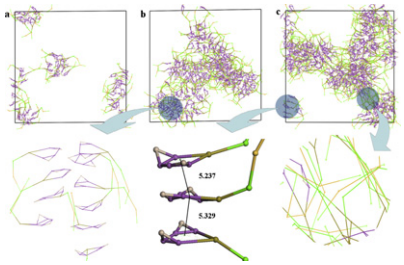
HIGHLIGHTS

- Simulation of gelation was expanded to large scale and long time by using CG-MD.
- We got the gel's configuration on molecular level (π stacking, entanglement).
- We confirmed the π–π stacking as the mainly gelation driven force.

GRAPHICAL ABSTRACT



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ABSTRACT

Fmoc protected D-Ala-D-Ala dipeptides were known to self-assemble into supramolecular hydrogel with interesting properties. However their molecular mechanisms were not well understood. In this study, a series of coarse grained molecular dynamics simulation were conducted to investigate the formation of this hydrogel at different concentrations. The three dimensional network of hydrogel and the stacking of the Fmoc planes were observed intuitively from the snapshots of the trajectory. Importantly, by analyzing the RDF of Fmoc planes' centriods and the distribution of neighboring Fmocs, we confirmed the π–π interaction as the mainly driving force for the gelation process.

1. Introduction

Hydrogel was composed of a three dimensional and cross linked network spanning the aqueous media [1]. They are everywhere in nature, such as the connective tissues in our body, the cornea in eyes, and other components of organisms [2]. The man-made hydrogels were treated as important biomaterials, and were widely used in tissue engineering [3], chemical sensing [4] and controlled drug delivery [5], as they have good biocompatible and biodegradable properties [6]. Also, they were easy to synthesize in large quantities and can be easily decorated as we need [7]. Those characteristics make it a research hotspot in recent years.

Specifically, in tissue engineering, hydrogel was frequently used as 3D scaffolds to support the growth of cultured cells because of their similarity to the natural extracellular matrix, which allows cell adhesion [6]. As for drug delivery, the nano-fibers formed by the self-assembly of hydrogelators entangled with each other lead to a 3D elastic network, which can encapsulate water and therapeutic agents. Even some hydrogelators themselves could serve as anti-inflammatory agents [8].

Supramolecular hydrogels were more favored for their outstanding features, such as, easy to modify, accessible to enzymes. They were formed by the self-assembly of small molecules with weak interactions (such as π–π interactions, hydrogen bonding, or electrostatic interactions) unlike the polymeric hydrogels which resulted from the cross-linking of polymer chains [9]. Vegners et al. reported the formation of supramolecular hydrogels with Fmoc-protected amino acids and dipeptides for the first time in 1995 [10]. During the process of synthesizing pyrene butyryl D-Ala-D-Ala as a short oligopeptidic hydrogelator, Xu and co-workers found that the intermediate, Fmoc-D-Ala-D-Ala, formed hydrogels efficiently

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