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Diverse stacking and facing directions of ß-strands alters the structural stability and mechanical properties of hIAPP protofibrils

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Amyloid protofibrils are mainly implicated to degenerative and neurodegenerative diseases such as type-2 diabetes, dialysis related diseases, Alzheimer's disease and Parkinson's diseases and so forth. Pathological characteristic of amyloid protein are not easily degraded under physiological condition which amyloid fibrils have high material properties. Based on these material characteristic, several research groups utilized amyloid fibrils as basic functional material template, which can be used in conductive nanowires, durg delivery carrier and nano structured biofilms etc. Recently, *in vitro* studies have been conducted to investigate the structural reaction and characteristic of amyloid proteins via force spectroscopy methods such as atomic force microscopy (AFM) and optical tweezers. However, computational methods are effectively revealing the mechanical properties of the amyloid protofibrils and provide structural information about the amyloids. In the present study, we reported the diverse material properties and behaviors based on different stacking and facing of polymorphic hIAPP segments using MD simulations and steered molecular dynamics (SMD) methods. From our results, we examined how these mechanical properties may differ with respect to the structural composition of beta strand segments.

Biography

Myeongsang Lee has completed his Bachelor's degree from Department of Mechanical Engineering, Dongguk University and completed his Doctoral studies in Korea, Department of Mechanical Engineering; Korea University, South Korea. He is majoring in protein engineering, especially in computational protein engineering using molecular dynamics. He has published 5 papers in reputed SCI (E) journals.

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