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Session: Simulation

An insight into fibre formation mechanisms through computer simulation

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Fibres formed by spontaneous self-assembly of small molecules, such as peptides, are key components of many foods: providing texture, stabilising formulations and influencing flow and processing properties. Also, naturally occurring “fibre” is central to a healthy diet, reducing the likelihood of diseases such as heart disease and diabetes, and generally improving digestive health. There are also various other situations in which spontaneously formed fibres can play either a favourable or an unfavourable role. Gels and some diseases, such as Alzheimer's disease, are examples from the two ends of this spectrum of fibre-related phenomena.

Whilst fibre formation is clearly ubiquitous, its microscopic origins and control mechanisms are not well understood. Here, therefore, we use Molecular Dynamics simulation of coarse-grained disc-shape particles to study the spontaneous initiation and growth of fibre structures from an amorphous solution. The effects of different parameters on the temperature-dependent process of fibre self-assembly are, thus, investigated. Through this, a pathway for the hierarchical formation of fibres is identified. Developing this understanding further, it is observed that adding small seeds into the system can induce fibre self-assembly at significantly higher temperatures. By shedding light on the mechanisms of self-assembly of fibres, this study provides useful insights for improved control of fibre-containing foods which should be of benefit to future process or product development.