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(POS-67) Frustrated Self-Assembly

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Biomolecular self-assembly lies at the very heart of the function of living cells, where it organizes individual components into functional biological machines. The macromolecular sub-units typically correspond to proteins, whose shapes have been optimized over millions of years of evolution to ensure a proper functionality of the self-assembled structures. However, in pathological cases, proteins fail to achieve the optimal folding, which often leads to **complex ill-fitting shapes**. This produces **geometrical incompatibility**, which leads to **frustrated interactions between the sub-units**. Surprisingly, despite a huge variability in protein structure, such misfolded units tend to **robustly self-assemble** into aggregates with **well-defined morphologies**. Interestingly, these structures display a **clear preference for slimmer topologies**, such as fiber aggregates. This emergent principle of **dimensionality reduction** suggests that the aggregation of irregular components derives from the **generic physical principles**, rather than the microscopic details of the interactions.

Inspired by this idea, we model the frustrated self-assembly of ill-shaped proteins as **coarse-grained anisotropic particles**, whose interactions depend on their relative orientations and positions in space. This simple model successfully **reproduces a hierarchy of aggregate morphologies** and gives pointers to the origins of dimensionality reduction.

Keyword-1

self-assembly

Keyword-2

frustration

Keyword-3

statistical models

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