The time complexity of self-assembly

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1. Abstract

The time efficiency of self-assembly is crucial for many biological processes. Moreover, with the advances in nanotechnology, time efficiency in artificial self-assembly has become ever more important. While structural determinants and the final assembly yield are increasingly well understood, kinetic aspects concerning time efficiency remain much more elusive. In computer science, the concept of time complexity is used to characterize the efficiency of an algorithm and describes how the algorithm's runtime depends on the size of the input data. Here we characterize the time complexity of nonequilibrium self-assembly processes by exploring how the time required to realize a certain, substantial yield of a given target structure scales with its size. We identify distinct classes of assembly scenarios, i.e., "algorithms," to accomplish this task and show that they exhibit drastically different degrees of complexity. Our analysis enables us to identify optimal control strategies for nonequilibrium self-assembly processes. Furthermore, we suggest an efficient irreversible scheme for the artificial self-assembly of nanostructures, which complements the state-of-the-art approach using reversible binding reactions and requires no fine-tuning of binding energies.