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Abstract

Using Patchy Particles to Shed New Light on the Autocatalytic Aggregation of Soft Matter †

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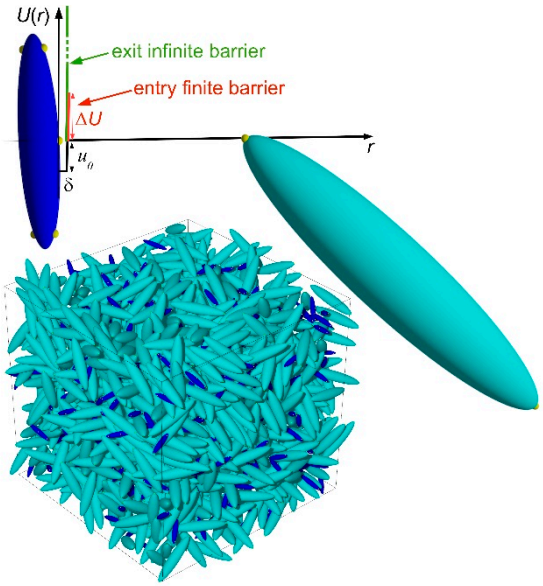
Autocatalysis, i.e., the speeding up of a reaction through the very same molecule which is produced, is common in chemistry, biophysics, and material science. Despite the pervasiveness of autocatalytic phenomena in nature and technology, autocatalytic aggregation has so far remained out of reach of realistic numerical simulations. Rate-equation-based approaches are often used to model the time dependence of products, but the key physical mechanisms behind the reaction cannot be properly recognized and then taken into account. On the contrary, patchy particles are designed learning from nature and can be thought of as an archetype of real monomers, but so far they completely lack autocatalysis. Here, building on previous studies on the subject [1–4], we report on a patchy particle model inspired by a bicomponent reactive mixture and endowed with adjustable autocatalytic ability [5]. Such a coarse-grained model captures all general features of an autocatalytic aggregation process that takes place under controlled and realistic conditions, including crowded environments. Simulation reveals that a full understanding of the kinetics involves an unexpected effect that eludes the chemistry of the reaction, and which is crucially related to the presence of an activation barrier. The resulting analytical description can be exported to real systems, as confirmed by experimental data on epoxy–amine polymerizations, solving a long-standing issue in their mechanistic description.



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