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Dynamic self-assembly of chemically-propelled nanoscale building blocks YANPING CHEN, YUNFENG SHI, Rensselaer Polytechnic Institute — Self-assembly technique offers spontaneous, massively-parallel structure formation from bottom-up. So far, most research efforts have been focused on static self-assembly that is thermally driven towards a thermodynamic equilibrium. Less attention has been paid to dynamic self-assembly that evolves to a non-equilibrium steady state under a dissipative driving force. This project aims to investigate the non-equilibrium self-assembly behaviors of chemically-propelled nanoscale building blocks via molecular dynamics simulations. We utilize a catalytic building block, that has been shown, when isolated, to exhibit self-motile behavior when immersed in a fuel environment. Upon increasing the number density of the building blocks, interesting collective behaviors emerge due to direct interactions between the building blocks or indirect interactions via the fuel environment. The simulation system is also subjected to an artificial operation of converting products back to fuel molecules. The heat generated by the exothermic chemical reaction will also be removed. In this way, a steady-state, as well as the resulting dynamic self-assembly pattern, can be obtained.

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