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Molecular design of self-propelled building blocks for dynamic self-assembly YUNFENG SHI, YANPING CHEN, Rensselaer Polytechnic Institute — Our research focuses on molecular design of self-propelled nanoscale objects serving as basic building blocks for dynamic self-assembly. Unlike static self-assembly which is driven thermally towards equilibrium, dynamic self-assembly evolves to a non-equilibrium steady state under a dissipative driving force. In this work, we use reactive molecular dynamics simulations to investigate how catalytic chemical reactions drive the motion of nanoscale building blocks. A fuel-catalyst reactive potential based on the reactive-state summation (RSS) scheme is designed for a model exothermic reaction. By strategically placing catalysts on the nanoscale building-blocks, asymmetric chemical reactions can be achieved which stimulate linear or rotational motion of the building-blocks. The observed propulsion can be understood in terms of momentum transfer. Importantly, the conversion efficiency from chemical to mechanical work is analyzed and used as an optimization target for molecular design of the chemically propelled building blocks.

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