

Evolutionary Design of Self-assembling Chemical Systems

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Abstract

Ligation is a form of chemical self-assembly that involves dynamic formation of strong covalent bonds in the presence of weak k associative forces. We study an extremely simple form of ligation by means of dissipative particle dynamics (DPD) model extended to include the dynamic making and breaking of strong bonds, which we term dynamically-bonding dissipative particle dynamics (DDPD). Then we use a chemical genetic algorithm (CGA) to optimize the model's parameters to achieve ligation of trimers - a proof of principle for the evolutionary design of self-assembling chemical systems.