Design Principles for Self-assembly of Similar Molecules

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CONTENTS

S1. The nonbonded interaction parameters of coarse-grained models .................................................................3

S2. The bonded interaction parameters of coarse-grained models......................................................................3

S3. The morphology evolution processes of three times simulations during the first step simulation .........................3

S4. The morphology evolution processes of three times simulations during the second step simulation ..................3
S1. The nonbonded interaction parameters of coarse-grained models

Table S1. The nonbonded interaction parameters between two coarse-grained beads

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Figure S1. The bonded interaction parameters of s-AP\textsubscript{O} (a), s-AP\textsubscript{N} (b), m-AP\textsubscript{O} (c), m-AP\textsubscript{N} (d), s-BP\textsubscript{O} (e), and s-BP\textsubscript{N} (f). Because all the bond lengths and some angles have a very small fluctuation, which are regarded as constants, they require a large stiffness coefficient. At the same time, the stability of the overall molecular structure energy is required, therefore, the maximum value of $k_b$ and $k_a$ are set to be 10000 kcal/mol and 200 kcal/mol after trying.
S3. The morphology evolution processes of three times simulations during the first step simulation
Figure S2. The morphology evolution processes of s-AP$_O$ (a), s-AP$_N$ (b), m-AP$_O$ (c), m-AP$_N$ (d), s-BP$_O$ (e), and s-BP$_N$ (f) during the first step simulation.
S4. The morphology evolution processes of three times simulations during the second step simulation
Figure S3. The morphology evolution processes of s-AP\(_O\) (a), s-AP\(_N\) (b), m-AP\(_O\) (c), m-AP\(_N\) (d), s-BP\(_O\) (e), and s-BP\(_N\) (f) during the second step simulation (fusion step).