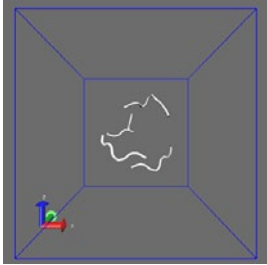
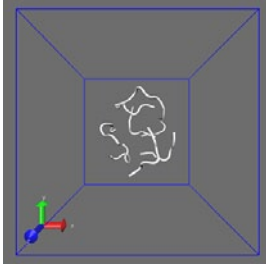
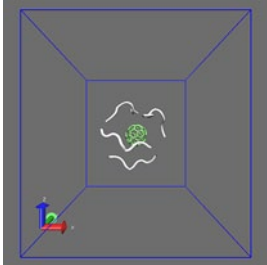
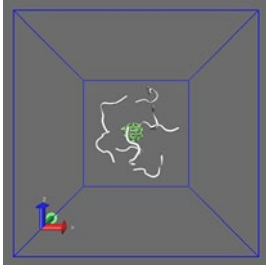
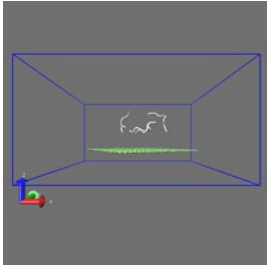
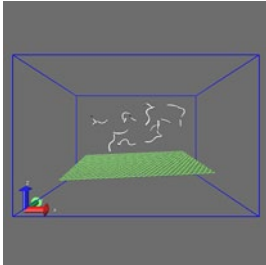


Table S1. Detailed information for the initial configuration of each system.

System	Terms	4 peptides	8 peptides
Pep	PBC (\AA^3)	51.04×55.23×53.00	52.03×52.87×55.97
	General view		
Pep+C ₆₀	PBC (\AA^3)	46.64×53.03×50.12	58.58×62.24×58.91
	General view		
Pep+Gra	PBC (\AA^3)	92.21×92.77×49.00	96.13×78.98×63.09
	General view		
Pep+SWCNT	PBC (\AA^3)	46.11×51.07×53.00	66.46×58.08×58.91
	General view	