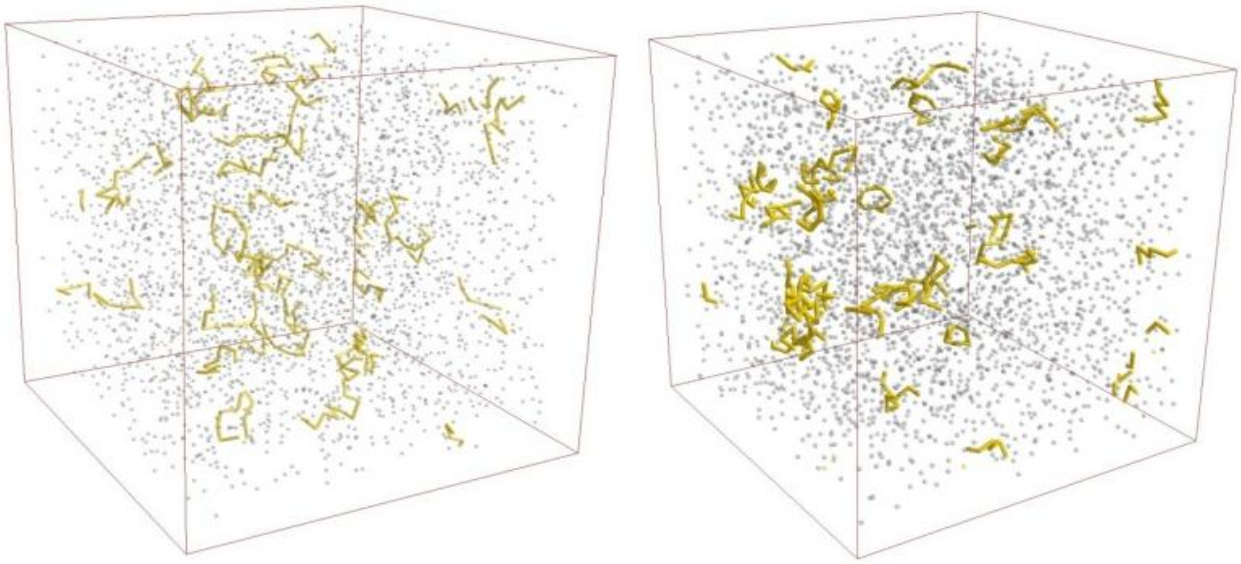
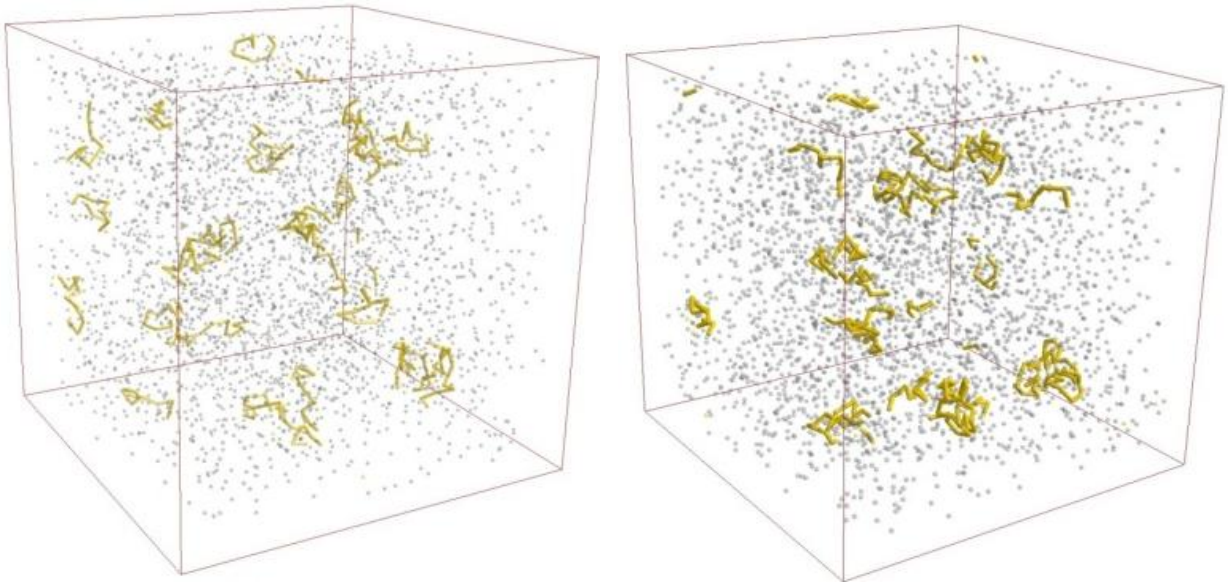
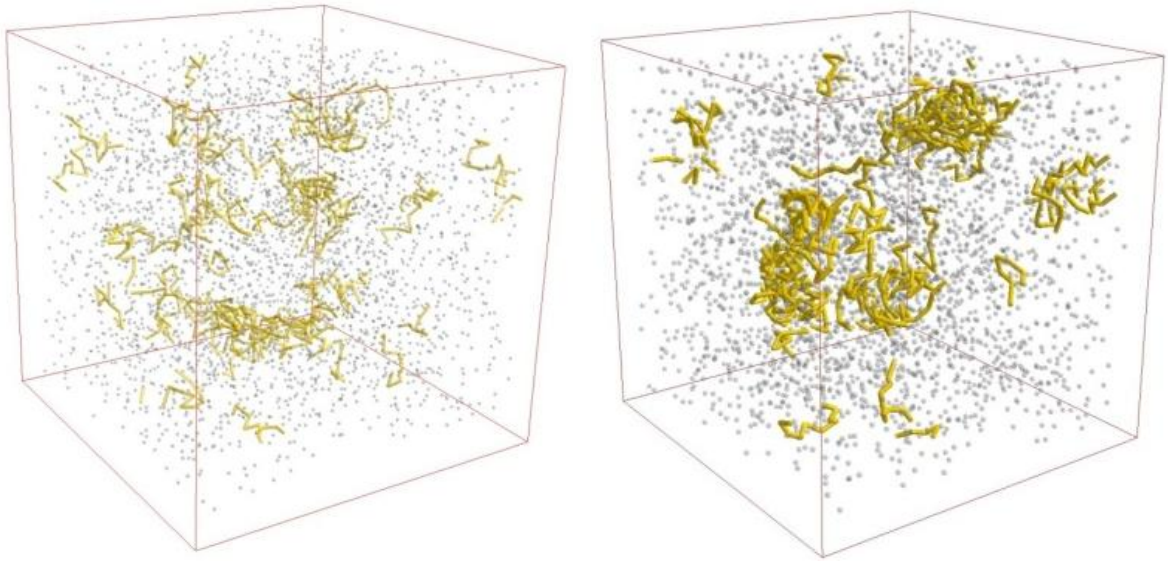


C_K = 0.01, C_{Ph} = 0.1, ε_{KPh} = -0.5

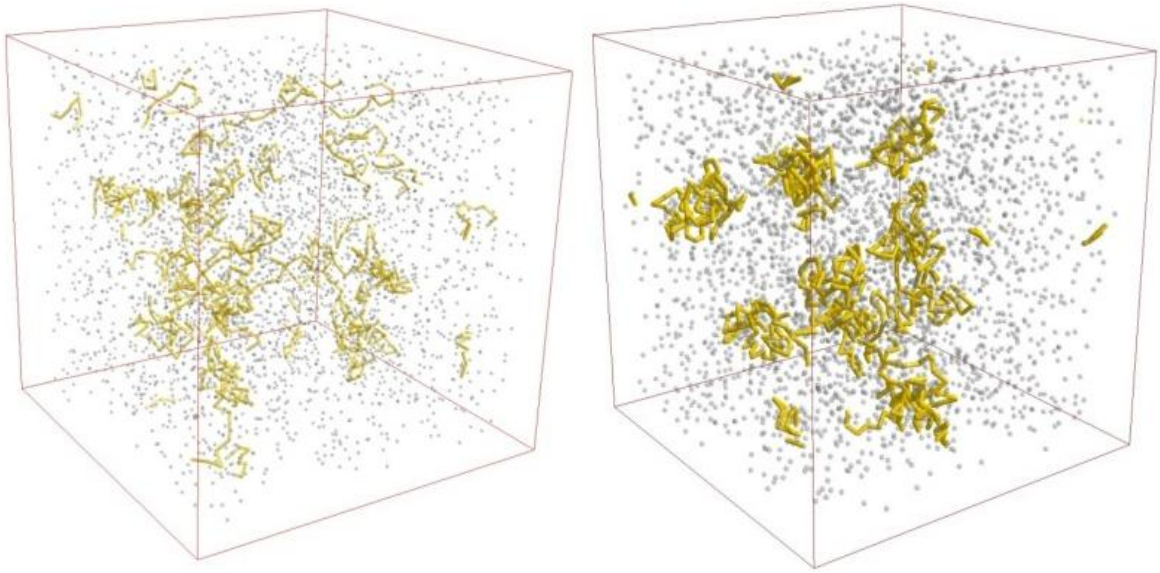


C_K = 0.01, C_{Ph} = 0.1, ε_{KPh} = -0.6

Figure S1. Endpoint snapshots of simulations of a 64^3 lattice size and either t = 10^5 MCS (left) or t = 10^6 MCS (right). The lysine (C_K) and phosphate (C_{Ph}) concentrations and the lysine-phosphate interaction strength (ε_{KPh}) for each row of simulation snapshots is shown below. Visually, peptides in snapshots at t = 10^6 are more aggregated than at t = 10^5, demonstrating that a total of 10^5 time steps is insufficient for system to reach an equilibrium.

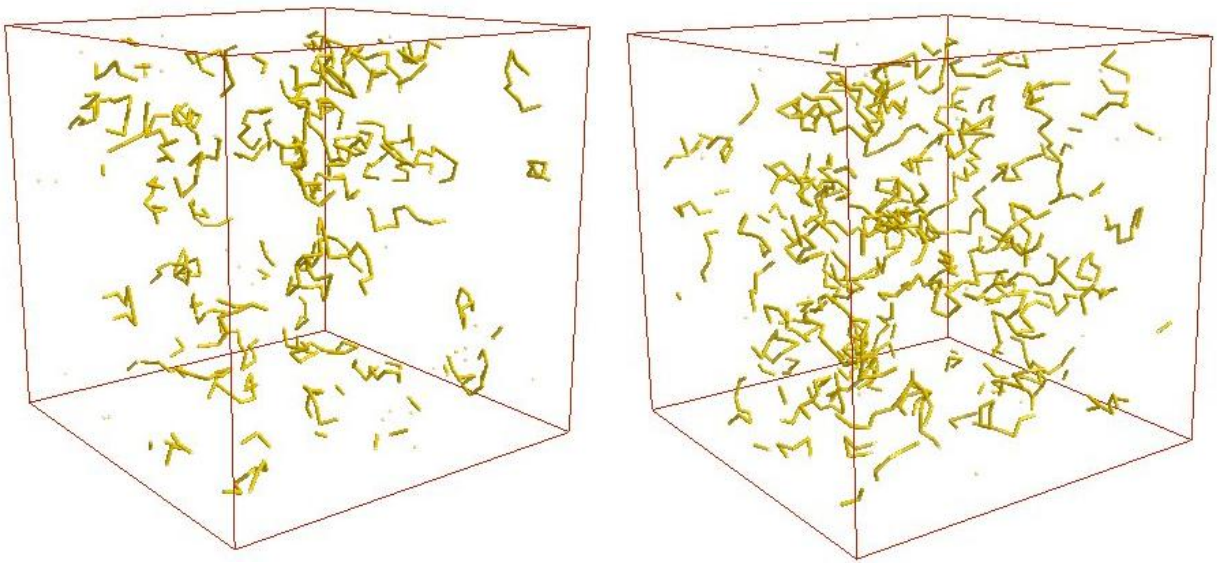


C_K = 0.02, C_{Ph} = 0.1, ε_{KPh} = -0.5

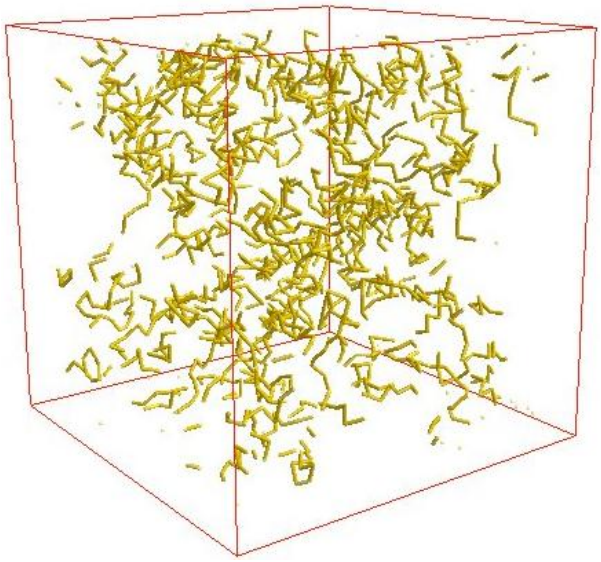


C_K = 0.02, C_{Ph} = 0.1, ε_{KPh} = -0.6

Figure S1 continued. Endpoint snapshots of simulations of a 64^3 lattice size and either t = 10^5 MCS (left) or t = 10^6 MCS (right). The lysine (C_K) and phosphate (C_{Ph}) concentrations and the lysine-phosphate interaction strength (ε_{KPh}) for each row is shown on the left. Visually, peptides in snapshots at t = 10^6 are more aggregated than at t = 10^5, demonstrating that a total of 10^5 time steps is insufficient for system to reach an equilibrium.



C_K = 0.2, ε_{KPh} = -0.5 C_K = 0.3, ε_{KPh} = -0.6



C_K = 0.5, ε_{KPh} = -0.7

Figure S2. Snapshots of simulations of a 64^3 lattice size and at the end of time step t = 10^6 MCS. Simulations do not contain phosphate. The lysine (C_K) concentrations and lysine-phosphate interaction strength (ε_{KPh}) are shown below each snapshot.

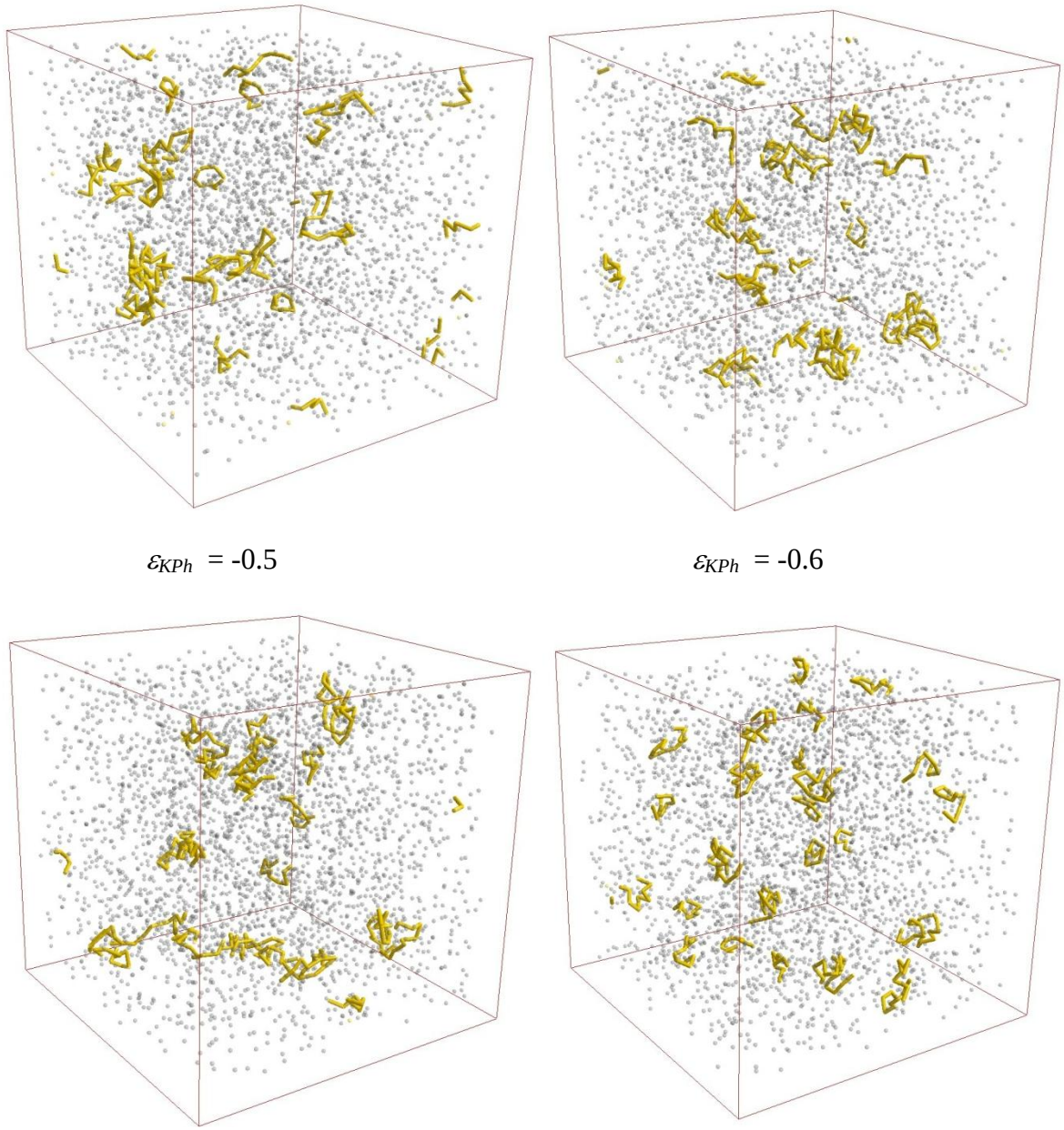


Figure S2 continued. Snapshots of simulations of a 64^3 lattice size and at the end of time step t = 10^6 MCS. The lysine (C_K) and phosphate (C_{Ph}) concentrations were 0.01 and 0.1, respectively. The lysine-phosphate interaction strength (ε_{KPh}) is shown below each snapshot.

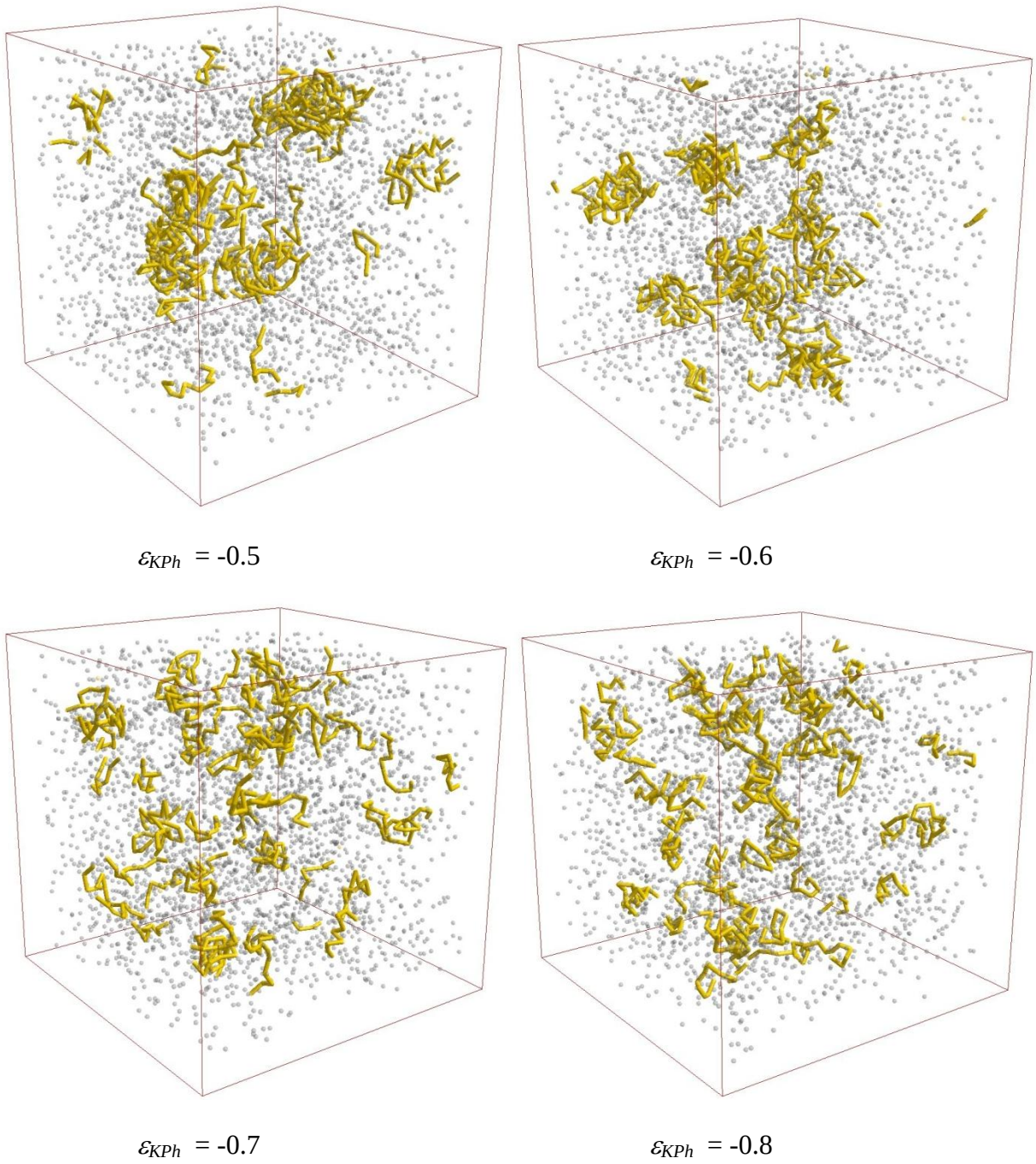
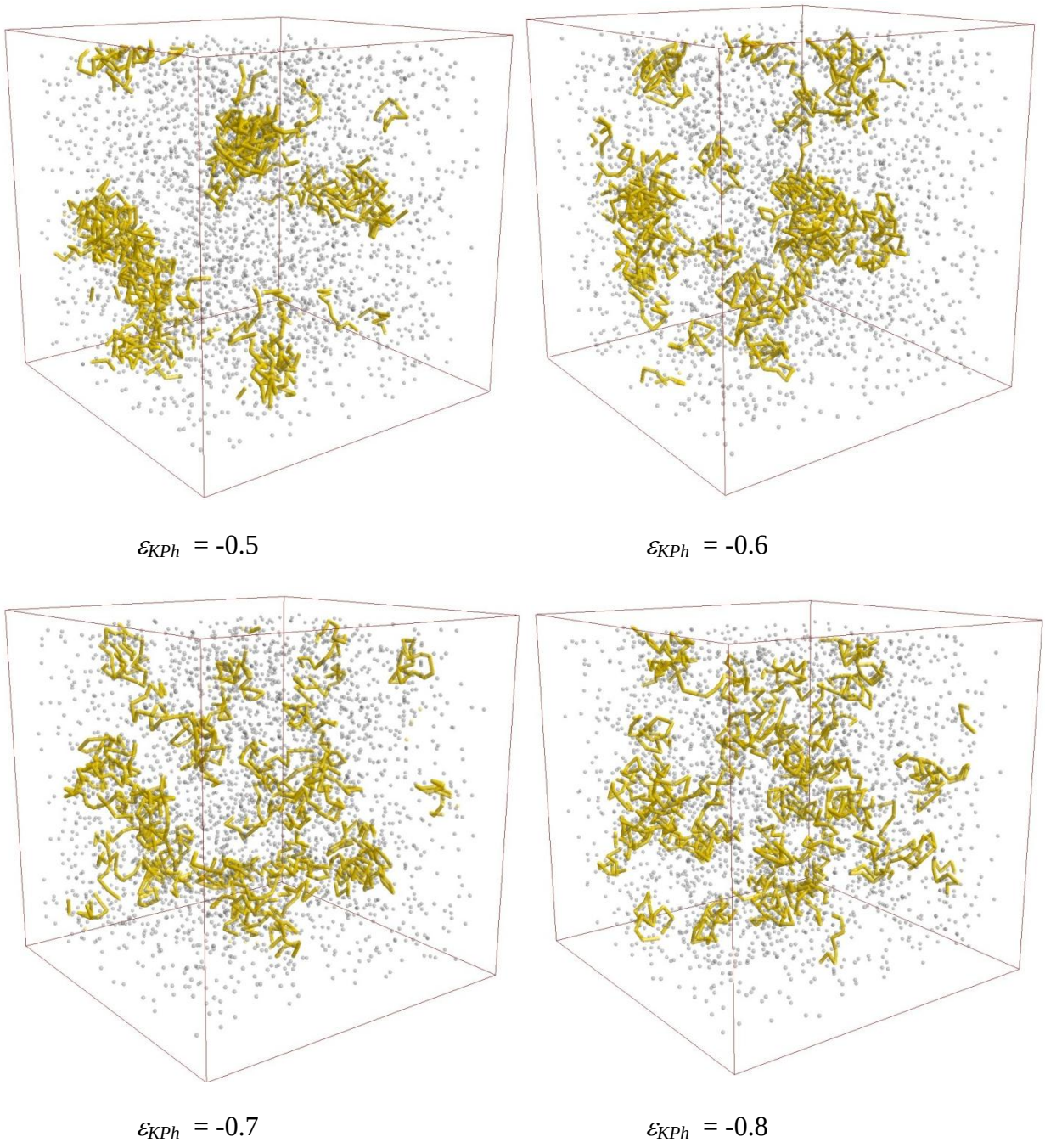


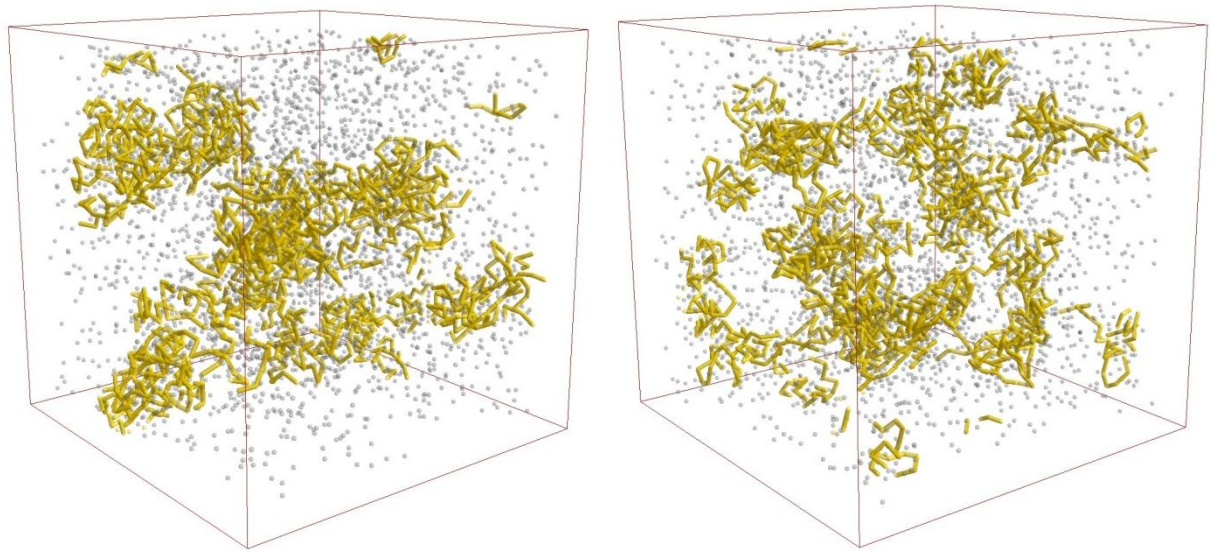
Figure S2 continued. Snapshots of simulations of a 64^3 lattice size and at the end of time step t = 10^6 MCS. The lysine (C_K) and phosphate (C_{Ph}) concentrations were 0.02 and 0.1, respectively. The lysine-phosphate interaction strength (ε_{KPh}) is shown below each snapshot.



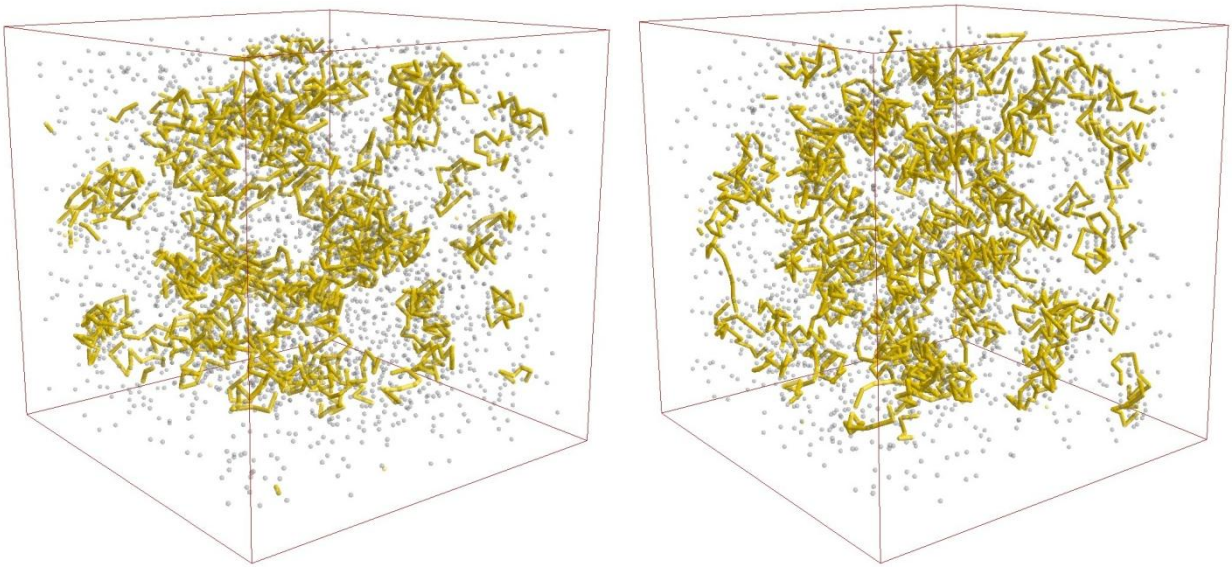
ε_{KPh} = -0.5 ε_{KPh} = -0.6

ε_{KPh} = -0.7 ε_{KPh} = -0.8

Figure S2 continued. Snapshots of simulations of a 64^3 lattice size and at the end of time step t = 10^6 MCS. The lysine (C_K) and phosphate (C_{Ph}) concentrations were 0.03 and 0.1, respectively. The lysine-phosphate interaction strength (ε_{KPh}) is shown below each snapshot.

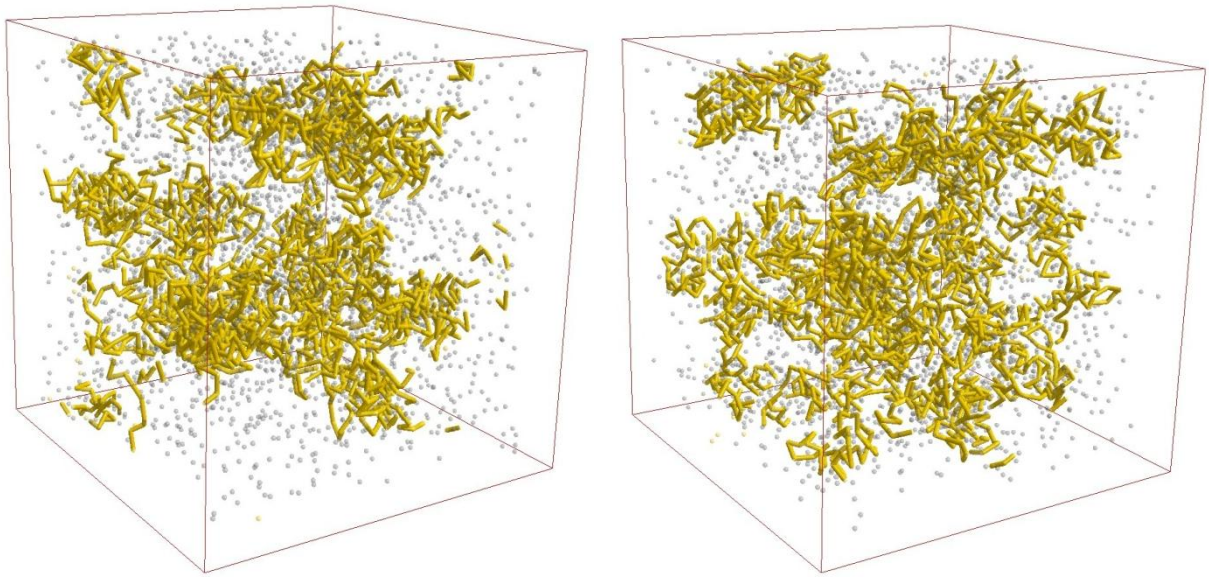


ε_{KPh} = -0.5 ε_{KPh} = -0.6

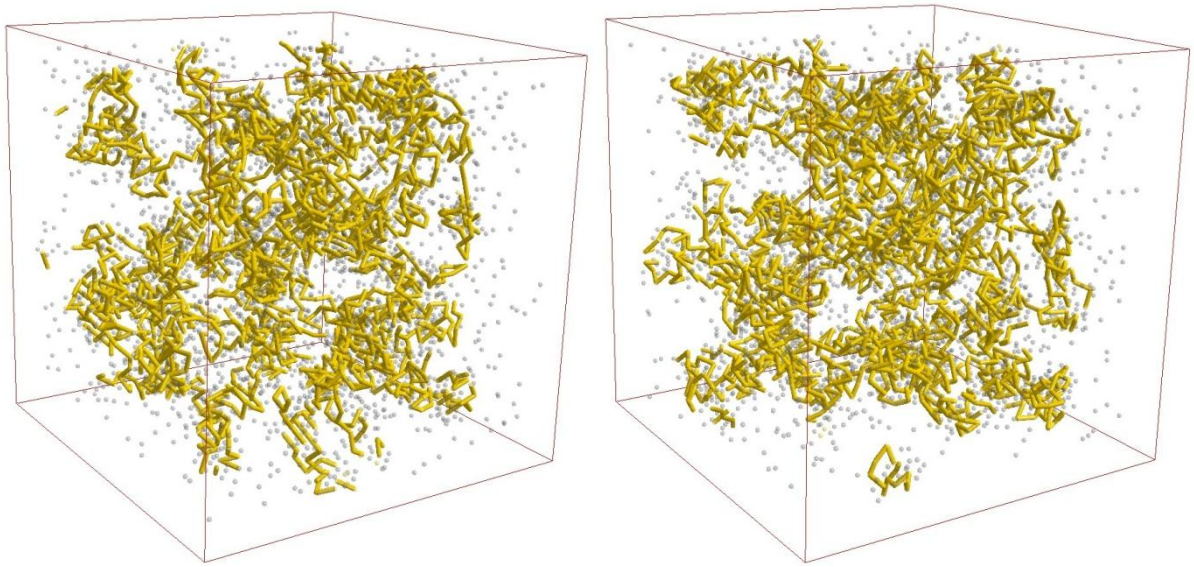


ε_{KPh} = -0.7 ε_{KPh} = -0.8

Figure S2 continued. Snapshots of simulations of a 64^3 lattice size and at the end of time step t = 10^6 MCS. The lysine (C_K) and phosphate (C_{Ph}) concentrations were 0.05 and 0.1, respectively. The lysine-phosphate interaction strength (ε_{KPh}) is shown below each snapshot.



ε_{KPh} = -0.5 ε_{KPh} = -0.6



ε_{KPh} = -0.7 ε_{KPh} = -0.8

Figure S2 continued. Snapshots of simulations of a 64^3 lattice size and at the end of time step t = 10^6 MCS. The lysine (C_K) and phosphate (C_{Ph}) concentrations were 0.07 and 0.1, respectively. The lysine-phosphate interaction strength (ε_{KPh}) is shown below each snapshot.